01 SOLID FUELS

Sources, winning, properties

13/00629 A study of chemical structure changes of Chinese lignite during fluidized-bed drying in nitrogen and air

Tahmasebi, A. *et al. Fuel Processing Technology*, 2012, 101, 85–93.

A Chinese lignite coal was dried in a fluidized-bed reactor in the presence of air and nitrogen to examine the effect of temperature, particle size, gas flow rate, and sample mass. The changes of chemical structure during drying were investigated using FTIR technique. The drying rate is shown to increase with increasing drying temperature and gas flow rate, and decreasing particle size. It has been found that the aliphatic hydrogen absorbance decreased with increasing drying temperature. These changes in aliphatic absorption were more significant after drying in air compared to in nitrogen. In air drying the absorption of oxygen-containing functional groups increased gradually with increasing temperature up to 200 °C and declined thereafter due to the decomposition of these groups to release CO and CO_2 or react with nearby hydroxyl groups to produce esters. Carbonyl groups decreased progressively with temperature in nitrogen while carboxylate and aromatic carbon absorption increased up to 250 °C and decreased thereafter. During air drying, the aromatic carbon absorption remained relatively unchanged suggesting the reaction of aliphatic groups with oxygen may be a primary oxidation mechanism.

13/00630 Advanced characterization of physical properties of coals with different coal structures by nuclear magnetic resonance and X-ray computed tomography

Li, S. *et al. Computers & Geosciences*, 2012, 48, 220–227.

In order to understand the correlation between coal structure and physical property of coal, samples with different coal structures were collected from the Late Permian period coal seams in the Laochang area, Yunnan Province, China. A set of experiments were carried out to quantitatively characterize the physical properties of coals with different coal structures using advanced and non-destructive low-field nuclear magnetic resonance (NMR) and X-ray computed tomography (X-CT). The experimental results gave us confidence to conclude that the evolution of the coal structures can be divided into five stages with stress increasing: the fractures closing stage, the microfractures development stage, the cracks development stage, the shear deformation stage, and the plastic deformation stage. Each stage corresponds to a different coal structure with unique physical characteristics. The undeformed coal is dominated with pores and a small amount of poorly connected fractures. In the proto-cataclastic stage, the volume of the mesopores, macropores and fractures sharply decreases with stress increasing. The coal rock becomes more compacted. Additionally, the connectivity between fractures and pores becomes worse. The cataclastic coal has well-developed mesopores, macropores and fractures but few micropores and transition pores. The connectivity between fractures and pores is most conducive to the exploitation of coalbed methane. In the mylonitic coal stage, the plastic deformation occurs, resulting in the reduction and discontinuity of mesopores, macropores, and fractures. Moreover, the undeformed coal has the best homogeneity, and the mylonitic coal has the highest heterogeneity, resulted from the uneven distribution of the maceral, pores, fractures, and minerals caused by later stress effect. Furthermore, the CT porosities have a good positive correlation with the permeability; the average CT number, the standard deviation of CT number have a negative correlation with the permeability.

13/00631 Analysis on rock burst danger when fully-mechanized caving coal face passed fault with deep mining

Chen, X. *et al. Safety Science*, 2012, 50, (4), 645–648.

When fully-mechanized caving face passed fault, rock burst accidence easily occurred. The SOS microseism monitoring system was applied to monitor the microseismic activities all time occurred in the coal and rock mass near the fault area. Variation features of microseismic energy releasing and microseismic frequency were analysed. Numerical simulation method was used to research the abutment stress distribution when coal face passed fault, which was compared with microseism occurrence rules. When the coal face approached to fault, the abutment stress increases gradually, so the high stress would accumulate near the fault region. When the coal face left fault, the abutment stress decreased. The SOS microseism monitoring results showed that microseismic activity in the fault area had a high instability. When the coal face neared to the fault, total energy value and frequency released by the microseism steadily increased. The maximum energy peak value also had the tendency to rapidly increase. Before the strong shock occurred, there was a period of weak seismic activity. The weak seismic activity showed energy accumulation for strong shock, which can be used to forecast the danger of rock burst.

13/00632 Coal petrology and genesis of Jurassic coal in the Ordos Basin, China

Ao, W. *et al. Geoscience Frontiers*, 2012, 3, (1), 85–95.

Multiple sets of thick coal beds characterized by simple structure and shallow burial depth were developed in the Early and Middle Jurassic strata of the Ordos Basin, north-western China. The huge reserves of this high quality coal have a high commercial value. The authors studied the coal's petrologic characteristics and its maceral distribution to determine the maceral's contribution to generation of oil and gas. The results show that the Jurassic coals in the Ordos Basin have special petrological features because of the Basin's unique depositional environment which was mainly a series of high-stand swamps in the upper fluvial system. These petrographic features are a result of the development of typical inland lakes where some sand bodies were formed by migrating rivers. After burial, the peat continued to undergo oxidizing conditions, this process generated extensive higher inertinite contents in the coals and the vitrinite components were altered to semi-vitrinite. The macroscopic petrographic types of these Jurassic coals are mainly semi-dull coal, dull coal, semilustrous and lustrous coal. The proportions of semi-dull coal and dull coal are higher in the basin margins, especially in the area near the northern margin. The numbers of semilustrous and lustrous coals increase southwards and towards the central basin. This situation indicates that different coal-forming swamp environments have major controlling effects on the coal components. Another observation is that in the Ordos' coal sequences, especially in the lower part, some sandstone beds are thick, up to 20 m with a coarse grain size. The higher fusinite content in the macerals accompanies a higher semi-vitrinite content with more complete and regular plant cell structure. The fusinite structure is clear and well preserved. After burial, the lithology of the roof and floor rocks can continue to affect the evolution of coal petrology. The sand bodies in the roof and floor exhibit good physical conditions so that pore water can maintain a long-term state of oxidation, circulation and connection to the coal. So coal components remain in an oxidation environment for a long time. Conversely, in the basin centre, lacustrine facies developed and peat was rapidly covered by mudstone after burial and subsequent coal beds rapidly entered a reducing environment. As a result, abundant gelatification occurred and the vitrinite content increased. Exinite often accumulated in a specific position in the coal bed. Although the average exinite content is not high on the whole, it does significantly contribute to the total hydrocarbon generation. The exinite content has been underestimated, especially the amorphous bituminous fluid and its importance is emphasized here. The reason is that the fluid flows easily into fusinite which has strong rigidity, or flows into some fissures, where it is commonly neglected.

13/00633 Experimental characterization of CH_4 release from coal at high hydrostatic pressure

Gal, N. L. *et al. International Journal of Coal Geology*, 2012, 96–97, 82–92.

Coal mines naturally emit gases, mostly methane, during exploitation and at the beginning of flooding. Once they are flooded, the conditions of gas migration are changed, and the capacity of release and retention of gas by coal is poorly known. The experimental device CASPER has made it possible to demonstrate and quantify a significant release of methane from coal under more than 3 MPa of hydrostatic pressure. The analysis of these results showed that the main fraction of released methane comes from sorption sites. The porous volume has a minor role in reaching content equilibrium, but has a strong effect on hydrostatic pressure, due to water penetration into the coal structure.

13/00634 Experimental study on oxygen consumption rate of residual coal in goaf

Qin, Y. *et al. Safety Science*, 2012, 50, (4), 787–791.

In order to research the actual oxygen consumption rate of residual coal in goaf, the heating and oxidizing experiment was conducted respectively on five types of single particle size of coal samples and one hybrid particle size of coal samples by using self-developed CSC-B2 test system. This study measured inlet and outlet oxygen concentration of the oxidation tank, and calculated the oxygen consumption rate of each coal sample at different temperatures. For the residual coal in the same goaf, which is regarded as a hybrid particle size of coal consisting of a variety of single granularity of coal, its oxygen consumption rate is the mass weighted average of the rate of each particle size of coal. Accordingly, this paper established the equation of oxygen consumption rate of hybrid particle size of coal samples, taking into account temperature, granularity and oxygen concentration. Then comparison between the calculated value and the actually measured value of oxygen consumption rate of hybrid particle size of coal samples at different temperatures was conducted. And the results reveal that the calculated value basically coincide with the actually measured one. Moreover, the results prove that the established calculation formula for oxygen consumption rate can be used to accurately calculate the actual oxygen consumption rate of residual coal samples. The achievement of this research is of theoretical and practical significance for learning about the characteristics of coal spontaneous combustion and forecasting the self-ignition of residual coal in goaf.

13/00635 Geomorphology of coal seam fires

Kuenzer, C. and Stracger, G. B. *Geomorphology*, 2012, 138, (1), 209–222.

Coal fires occur in underground natural coal seams, in exposed surface seams, and in coal storage or waste piles. The fires ignite through spontaneous combustion or natural or anthropogenic causes. They are reported from China, India, USA, South Africa, Australia, and Russia, as well as many other countries. Coal fires lead to loss of a valuable resource (coal), the emission of greenhouse-relevant and toxic gases, and vegetation deterioration. A dangerous aspect of the fires is the threat to local mines, industries, and settlements through the volume loss underground. Surface collapse in coal fire areas is common. Thus, coal fires are significantly affecting the evolution of the landscape. Based on more than a decade of experience with *in situ* mapping of coal fire areas worldwide, a general classification system for coal fires is presented. Furthermore, coal seam fire geomorphology is explained in detail. The major landforms associated with, and induced by, these fires are presented. The landforms include manifestations resulting from bedrock surface fracturing, such as fissures, cracks, funnels, vents, and sponges. Further manifestations resulting from surface bedrock subsidence include sinkholes, trenches, depressions, partial surface subsidence, large surface subsidence, and slides. Additional geomorphologic coal fire manifestations include exposed ash layers, pyrometamorphic rocks, and fumarolic minerals. The origin, evolution, and possible future development of these features are explained, and examples from *in situ* surveys, as well as from high-resolution satellite data analyses, are presented. The geomorphology of coal fires has not been presented in a systematic manner. Knowledge of coal fire geomorphology enables the detection of underground coal fires based on distinct surface manifestations. Furthermore, it allows judgments about the safety of coal fire-affected terrain. Additionally, geomorphologic features are indicators of the burning stage of fires. Finally, coal fire geomorphology helps to explain landscape features whose occurrence would otherwise not be understood. Although coal fire-induced thermal anomalies and gas release are also indications of coal fire activity, as addressed by many investigators, no assessment is complete without sound geomorphologic mapping of the fire-induced geomorphologic features.

13/00636 High quality of Jurassic coals in the southern and eastern Junggar coalfields, Xinjiang, NW China: geochemical and mineralogical characteristics

Li, J. *et al. International Journal of Coal Geology*, 2012, 99, 1–15.

The Junggar coal basin, with enormous coal reserves, is one of the largest coal basins in Xinjiang Province, north-west China. According to the exploration data, there is one to dozens of workable coal seams developed in the Xishanyao Formation of Middle Jurassic across the whole basin, with the maximum accumulated coal thickness of over 100 m. Ninety-six bulk coal samples from six exploration boreholes in the Southern and eastern Junggar coalfields were collected to investigate the coal qualities of the Junggar coals. The mineralogical characteristics of the studied coals were determined by powder X-ray diffraction and geochemical analyses are performed by means of inductively-coupled plasma atomic-emission spectrometry (ICP-AES) and inductively-coupled plasma mass spectrometry (ICP-MS). The eastern and southern Junggar bituminous coals are all characterized by low ash yields, low S contents, and low mineral contents. Furthermore, the concentrations of most major and trace elements in both the eastern and southern Junggar coals are relatively low with respect to other Chinese and worldwide coals, with the exceptions of Sr and Ba. The results show that elements including K, Li, Ti, Sc, V, Cr, Ga, Rb, Zr, Pb, and rare earth elements (REEs), have aluminosilicate affinities. Ca-bearing and Fe-bearing carbonate affinities are deduced for Ca, Mg, Fe, Mn, Sr and Ba. Sulfur (Fe), Zn, Pb, Cu and As show a partial sulfide affinity in some coals. An apatite and/or crandallite affinity is deduced from relatively high correlation of P, Sr and Ba. The very high coal quality of Junggar coals is attributed to very low detrital supply in very stable shallow-lake sedimentary facies during peat accumulation. Slight differences of peat bog accumulation rate, water table, and oxidizing-reducing condition account for the merging and splitting of coal seams in different coal exploration areas and the slight differences of mineral, S, ash, and trace element contents. In summary, the eastern and southern Junggar coals with very enormous reserves are characterized by high quality, which is significantly and environmentally relevant to coal combustion by-products (CCPs) and potential emissions of gaseous pollutants/particulate matter during the large coal consumption in pulverized coal combustion power stations in Xinjiang Province. The high coal quality of the Junggar coals is expected to generate CCPs that can be reused for various purposes with low environmental threat.

13/00637 Investigation into the nonlinear damage model of coal containing gas

Yang, X. *et al. Safety Science*, 2012, 50, (4), 927–930.

By taking the non-linear deformation properties of coal into consideration, the non-linear constitutive equation was founded. And in view of the compressible property of gas, the idea of compressive energy of gas was introduced. According to the continuous damage theory and mesoscopic damage theory, it is assumed that the damage variable has a power function relation with the porosity. By applying the thermodynamics energy conservation laws, a new non-linear damage constitutive model of coal containing gas was deduced, and the correctness of the new model was verified by comparing with the former experimental results. This model can provide theoretical reference for understanding and solving these dynamic gas disasters such as coal and rock outburst. Moreover, based on this theory, prevention and control measures will be adopted to deal with the dynamic gas disasters according to ever-changing mining conditions.

13/00638 Mineralogical and geochemical compositions of the coal in the Guanbanwusu mine, Inner Mongolia, China: further evidence for the existence of an Al (Ga and REE) ore deposit in the Jungar coalfield

Dai, S. *et al. International Journal of Coal Geology*, 2012, 98, 10–40.

Aluminium-hydroxide (boehmite and diaspore)-, Ga-, REY (rare earth elements and Y)-, and Al-rich Pennsylvanian Taiyuan Formation coals have previously been found in the Jungar and Daqingshan coalfields, Inner Mongolia, China. Gallium, REY, and Al are potentially extractable and usable elements in combustion residues derived from these coals. This paper reports new results on 50 bench samples of the No. 6 coal from the Guanbanwusu mine, Jungar coalfield, Inner Mongolia, and provides new data and evidence for the existence of an Al (Ga, REY) ore deposit in the unique Jungar coalfield. The No. 6 coal in the Guanbanwusu mine has a low rank ($R_{o,ran} = 0.56\%$) and a low-sulfur content ($S_{t,d} = 0.58\%$). The proportion of inertinite in the coal (56.7%; mineral-free basis) is higher than that of vitrinite (31%). The minerals in the coal are mainly represented by kaolinite, boehmite, and chlorite, along with variable proportions in some samples of calcite, ankerite, siderite, and goyazite. Boehmite, goyazite, and part of the kaolinite were derived from bauxite in the weathered surface of the sediment-source region. Ankerite, calcite, and siderite in the coal are of authigenic origin. The chlorite in the Guanbanwusu coals appears to have a chemical composition intermediate between cookeite and chamosite. This mineral mainly occurs as cell-fillings, also indicating an authigenic origin, and was probably derived from hydrothermal fluids. A new mineral phase mainly composed of Ti, Cl, and Fe is probably a Ti-bearing oxychloride or hydroxychloride. Compared to other Chinese coals and to world hard coals, the coal from the Guanbanwusu mine is enriched in Al_2O_3 (9.34%), P_2O_5 (0.126%), Li (175 μg/g), F (434 μg/g), Cl (1542 μg/g), Ga (12.9 μg/g), Sr (703 μg/g), and Th (12.9 μg/g), but has a lower SiO_2/Al_2O_3 ratio (0.74) due to the higher proportions of boehmite and goyazite in the coal. The major carrier of P_2O_5 and Sr is goyazite. Lithium mainly occurs in the chlorite (cf. cookeite), kaolinite, and possibly, to a lesser extent, illite. Fluorine in the coal has a major boehmite affinity, but a small proportion may also occur in the organic matter and chlorite. Gallium in the coal largely occurs in goyazite. Chlorine is independent of other elements in the coal, associated neither with moisture nor with organic matter, but possibly occurring in molecular form (Cl_2) and in the Ti-bearing oxychloride or hydroxychloride. Thorium in the coal occurs in the clay and accessory minerals, and was mainly derived from detrital materials of the source region. Rare earth elements and Y have a mixed (organic and inorganic) affinity, largely occurring in goyazite-group minerals and, to a lesser extent, boehmite and organic matter. Most coal benches and partings have either an L-type or H-type of REY enrichment, owing respectively to the weathered bauxite source region and groundwater effects. The Al_2O_3, Ga, REY and possibly Li in the Guanbanwusu coals, like those in coals from the Jungar and adjacent Daqingshan coalfields, are industrially useful metals that could potentially be recovered from the relevant coal combustion residues. It is suggested that, if Ga in ash > 50 μg/g, REY > 800–900 μg/g, $SiO_2/Al_2O_3 < 1$ (or $Al_2O_3 > 40\%$ in ash), and coal thickness > 5 m, the coal combustion residues would be expected to be suitably enriched in Al_2O_3 and can be considered for Al_2O_3, Ga, and REY recovery.

13/00639 Mineralogy and geochemistry of the coals from the Karmozd and Kiasar coal mines, Mazandaran province, Iran

Moore, F. and Esmaeili, A. *International Journal of Coal Geology*, 2012, 96–97, 9–21.

The Karmozd and Kiasar mines are two major coal-producing areas in the central Alborz coal-bearing field, northern Iran. This study focused on the mineralogy and geochemistry, with respect to the mode of occurrence of elements in feed coals and element partitioning during coal preparation. The low sulfur content in the coal seams indicates a non-marine origin, i.e. deposition in lacustrine and swamp environments. Detrital minerals in the coal seams are quartz, feldspar (albite and orthoclase), mica (muscovite and biotite), amphibole (hornblende) and kaolinite. Authigenic minerals include pyrite, calcite and chlorite. The contents of most elements are within the general worldwide ranges (with the exceptions of Mn, Co and Cr, in some coal seams). Correlation coefficients between elements and the ash yield identified four separate groups of elements. The sequential extraction results indicate that Al, Na, K, Zn, Cu and Co principally occur in the silicates, whereas Pb and Cr mainly occur in the organic fraction. Calcium and Mg display strong affinities to the carbonate phase, while Cd mainly occurs in the water soluble and organic fractions. The calculated removability index shows that the coal cleaning method in Zirab not only removes mineral matter and pyritic sulfur, but also reduces the content of most inorganic elements.

13/00640 Permeability increase in Bowen Basin coal as a result of matrix shrinkage during primary depletion

Mazumder, S. *et al. International Journal of Coal Geology*, 2012, 96–97, 109–119.

Matrix shrinkage in coal-seam gas reservoirs as a result of production, and the resultant impact on absolute permeability, is a current area of intense interest. A number of publications have documented the existence of this phenomenon. The exponential growth behaviour of coal seam permeability with reservoir pressure depletion has been observed previously at the Fairway wells in the San Juan basin. More recently, an exponential trend has also been confirmed for a group of 10 wells in a region northeast of Fairway. An increase in the absolute permeability of coal seam is a result of matrix shrinkage caused by gas desorption, which becomes a dominant factor on cleat permeability over the effective horizontal stress change during production. Bottom hole pressure recovery during shut-in periods can provide valuable data concerning the impact of coal seam gas production on reservoir permeability. Arrow Energy's historical production data, from the MGP field in the Bowen Basin, contains over 60 instances of data on pressure recovery during shut-in. These time lapse build-up periods have been analysed using the pseudo-pressure method in an effort to gain an understanding of the extent and effect of this phenomenon within the company's existing assets. The method is based on a pseudo pressure function that uses the adsorption isotherm and the relative permeability relations of the reservoir. The infinite acting radial flow regime was identified and the gradient was recorded on a semi log plot of the pseudo pressure versus dimensionless time. Results from these tests show multi fold increase in absolute permeability as a function of the estimated reservoir pressure.

13/00641 Rapid regional outburst elimination technology in soft coal seam with soft roof and soft floor

Zhao, F. *et al. Safety Science*, 2012, 50, (4), 607–613.

In order to solve the problems in outburst elimination of coal seams with outburst potential, methods of field testing, theoretical analysis and numerical simulation are employed in this study. It is found that the horizontal stress concentration surrounding coal unloading boreholes is the primary cause of the coal and gas blowouts in the process of the coal unloading and permeability improvement with high-pressure water jet. The results indicate that low borehole density and inefficient drainage are the main reasons for the occurrence of high outburst indices in the effeteness validation of regional measures to control outbursts. Based on numerical modelling results and onsite parameter testing, reasonable parameters such as borehole density are determined, and hydraulic fracturing is applied to improve coal seam permeability and relieve stress levels so as to eliminate regional outburst potential. The effect is significant in the field application, coal and gas blowout during the coal unloading period with high-pressure water jet is reduced dramatically, and the roadway development rate is increased by 48%. It is demonstrated that the gas drainage combined with the hydraulic fracturing, coal unloading with high-pressure water jet is a practical and effective technique for rapid elimination of coal and gas outburst potential in roadway development.

13/00642 Relationship between EMR and dissipated energy of coal rock mass during cyclic loading process

Song, D. *et al. Safety Science*, 2012, 50, (4), 751–760.

Dynamic collapses of deeply mined coal rocks are severe threats to miners. In order to predict the collapses more accurately using electromagnetic radiation (EMR), this paper researched the energy conversion mechanism in the damage process of coal rock mass, analysed its EMR and dissipated energy, and a relationship between which was established using the voltage amplitude of EMR signal and hysteresis loop generated in the loading and unloading cycles as a bridge; then a series of cyclic loading experiments using coal samples of Junde and Xinlu coal mines from Heilongjiang province were carried out, and EMR signal released during these cycles were collected. Results show that during a whole damage process of a sample, the cumulative values of EMR energy and corresponding dissipated energy (hysteresis loop area) well subject to the form of $y = a\ln(x) + b$, whose correlation coefficients are above 0.90, and EMR signals received by different frequency antenna seldom impacted on this relationship; the total EMR energy released from the whole failure process of the samples obtained from adjacent sampling point in same mining area are different to some extent, so are the dissipated energy; compared with cyclic loading for coal rock mass orderly with the peak loads of 5 and 10 kN previously, the dissipated energy of direct using that of 15 kN increase 17.8%, and EMR signal is more abundant; EMR energy received in each cycle increase steadily with the improvement of load level, and in a single loading and unloading cycle, sometimes it is very rich in the unloading phase, even more than the loading one.

13/00643 Use of GIS to discover potential coalfields in Yatagan–Milas area in Turkey

Sutcu, E. C. *et al. International Journal of Coal Geology*, 2012, 98, 95–109.

The study was aimed to produce potential coalfield map using geographic information systems (GIS) in the Milas–Yatagan Basin. Frequency ratio model was used to define the relationships between the coal occurrences and the selected variables which are significant for coal prospection. Formation, geologic age, lithology, rock types, depositional environment, distance to fault and slope data of the study area were used as variables. Frequency ratio values of the variables were calculated and assigned to variable's class attributes. All variable maps were summed according to the frequency ratio values of superposed pixels to calculate the probability index. The probability index values of the potential map were classified into five classes as very high, high, medium, low and very low probability areas. Finally, the potential map was compared with known coalfields in the Milas–Yatagan Basin and calculated distribution of the known coalfields on the probable areas.

Preparation

13/00644 Application of the modified water-only cyclone for cleaning fine coals in a Turkish washery, and comparison of its performance results with those of spiral and flotation

Hacifazlioglu, H. *Fuel Processing Technology*, 2012, 102, 11–17.

Water-only cyclone (WOC) is an autogenous medium cyclone which performs a gravity separation using water as a separating fluid. Modified water-only cyclones (MWOC) are presently being used for fine coal cleaning in only two washeries in Turkey. In this study, MWOC was designed, installed via local facilities, and then implemented for the treatment of fine coal. The effects of the major parameters of MWOC, such as cyclone diameter, vortex finder diameter and apex diameter, on washing performance were investigated in detail. Then, the results obtained through the MWOC under optimum conditions were compared with those obtained through spiral and flotation. The tests show that the MWOC produced clean coal equal in quality to that produced by the spiral and flotation machine. However, the clean coal yield of the MWOC is quite a bit lower than that of the spiral and flotation machine, and the reject contains a significant amount of combustible matter. In summary, it was concluded that the MWOC can be used in washeries for pre-enrichment due to its simple structure, easy-control features and lower operational costs.

13/00645 Biodesulfurization of coal with *Acidithiobacillus caldus* and analysis of the interfacial interaction between cells and pyrite

He, H. *et al. Fuel Processing Technology*, 2012, 101, 73–77.

In the present work, the acidophilic and thermophilic strain *Acidithiobacillus caldus* was used for biodesulfurizing coal and bioleaching coal pyrite. The surface characteristics of cells and minerals and the mineral transformation during the coal pyrite leaching process were investigated combined with zeta-potential, FT-IR spectroscopy, scan electronic microscopy and X-ray absorption near edge structure spectroscopy (XANES). The results showed that the coal pyritic desulfurization with *A. caldus* was about 47% and the total desulfurization was 19%. After processed by cells, there was clear corrosion on the pyrite surface. Coal pyrite and elemental sulfur-grown cells had more hydrophilic functional groups than thiosulfate-grown cells. During the coal pyrite leaching course, the elemental sulfur was the main sulfur speciation but no other secondary mineral components were detected.

13/00646 Desulphurization and deashing of oxidized fine coal by Knelson concentrator

Uslu, T. *et al. Fuel Processing Technology*, 2012, 101, 94–100.

In order to efficiently clean fine coals, enhanced gravity separators, such as Knelson concentrator, have been developed. Although the Knelson concentrator has not been applied yet in industrial scale for fine coal cleaning, different investigations have been conducted in recent years. In this study, an oxidized coal with high sulfur was subjected to cleaning process by Knelson concentrator after being classified into the size fractions of $-106\,\mu m$, $-300+106\,\mu m$ and $-500+300\,\mu m$. Experimental variables were coal particle size, bowl speed and fluidizing water pressure. Maximum combustible matter recovery, pyritic sulfur rejection, and ash rejection were achieved to be 99.13%, 91.60%, and 60.94%, respectively. The highest separation efficiency for the pyritic sulfur and ash was determined to be 67.91% and 39.53%, respectively. These corresponded to the removal of 70.45% of pyritic sulfur with combustible matter recovery of 97.46% and removal of 45.96% of the ash with combustible matter recovery of 93.57%. Coal particle size, bowl speed and fluidizing water pressure were determined to affect the separation performance with a close interaction between them.

13/00647 Discrete element model for coal wellbore stability

Zhao, H. *et al. International Journal of Rock Mechanics and Mining Sciences*, 2012, 54, 43–46.

Coal-bed methane (CBM) is a significant component of unconventional natural gas production. As the world's natural gas demand grows, CBM exploration and development will become increasingly important for ensuring adequate natural gas supplies. To maximize the production of CBM in some complicated geological settings, it is becoming common practice to drill directional and horizontal wells in coal-beds; because of the special mechanical properties of the often fractured coal, the wells are prone to wellbore instability problems induced by drilling, completion and production operations. Considering the naturally cleated coal-bed, stress analysis has been conducted on the matrix blocks prone to slippage and a block analysis model for collapse pressure is established through equilibrium conditions of stresses. It was found from the block analysis model that increasing borehole pressure can increase or reduce wellbore stability, which depends on borehole size, cleat spacing, friction angle of cleat, cleat angle and the angle between block and the principal stress. Safe mud weights are calculated in three scenarios ($c > 0$, $c < 0$ and c swings between positive and negative). It was found that collapse position is sensitive to borehole size, and collapse pressure does not change much with borehole size.

13/00648 Effective removal of sulfur from high-sulfur coal prior to use by dry chlorination at low temperature

Shen, S. *et al. Journal of Hazardous Materials*, 2012, 217–218, 116–122.

Desulfurization of high-sulfur coal prior to use by dry chlorination under various conditions was investigated. The contents of total carbon, total sulfur, pyritic sulfur, sulfate and organic sulfur of the coal were 72.48, 5.95, 1.08, 0.66 and 4.22 wt%, respectively. It was found that the chlorination temperature and particle size had a great influence on sulfur removal. The optimal chlorination temperature and particle size for sulfur removal was 350 °C and 48–75 μm, respectively. Under optimal conditions, sulfur content in the chlorinated coal was 1.12 wt%. The removal percentages of total sulfur, pyritic sulfur, sulfate and organic sulfur were 67.7, 93.0, 65.6 and 61.6, respectively, indicating that a high proportion of organic sulfur, pyritic sulfur and inorganic sulfur were removed by dry chlorination. Meanwhile, the fixed carbon did not lose appreciably. It was speculated that the removal of organic sulfur by dry chlorination at 350 °C proceeded mainly based on the equation $2R\text{–}S + Cl_2 = 2R\text{–}Cl + S_2Cl_2$. The chlorinated coal thus obtained could be used in production of various carbon-containing materials such as metallurgical coke after a complete dechlorination pretreatment at 500–600 °C.

13/00649 Iron ore as oxygen carrier improved with potassium for chemical looping combustion of anthracite coal

Gu, H. *et al. Combustion and Flame*, 2012, 159, (7), 2480–2490.

Chemical looping combustion (CLC) is an innovative combustion technology with inherent separation of CO_2 without energy penalty. When solid fuel is applied in CLC, the gasification of solid fuel is the rate-limiting process for *in situ* gasification of coal and reduction of oxygen carrier. The K_2CO_3-decorated iron ore after calcinations was used as oxygen carrier in CLC of anthracite coal, and potassium ferrites were formed during the calcinations process. The experiments were performed in a laboratory fluidized bed reactor with steam as a gasification medium. Effects of reaction temperature, K_2CO_3 loading in iron ore and cycle on the gas concentration, carbon conversion, gasification rate and yields of carbonaceous gases were investigated. The carbon gasification was accelerated during the fast reaction stage between 860 and 920 °C, and the water–gas shift reaction was significantly enhanced in a wider temperature range of 800–920 °C. With the K_2CO_3 loading in iron ore increasing from 0% to 20% at 920 °C, the carbon conversion was accelerated in the fast reaction stage, and the fast reaction stage became shorter. The yield of CO_2 reached a maximum of 94.4% and the yield of CO reached a minimum of 3.4% when use the iron ore loaded with 6% K_2CO_3. SEM analysis showed that the K_2CO_3-decorating in iron ore would cause a sintering on the particle surface of oxygen carrier, and the K_2CO_3 loading in iron ore should not be too high. Cycle experiments indicate that the K_2CO_3-decorated iron ore has a relative stable catalytic effect in the CLC process.

13/00650 Mining-induced strata stress changes, fractures and gas flow dynamics in multi-seam longwall mining

Guo, H. *et al. International Journal of Rock Mechanics and Mining Sciences*, 2012, 54, 129–139.

This paper presents key findings from a recent comprehensive study of longwall mining-induced strata movement, stress changes, fractures, and gas flow dynamics in a deep underground coal mine in Anhui, China. The study includes field monitoring of overburden displacement, stress and water pressure changes at the longwall panel 1115 of the Guqiao mine. In addition, three-dimensional modelling of strata behaviour at the longwall panel using a three-dimensional finite element code and goaf gas flow simulations with a CFD code are carried out. This research has resulted in many new insights into the complex dynamic interaction between mining induced strata stress changes, fractures, and gas flow patterns. Based on the findings from the field monitoring and numerical modelling, a three-dimensional annular-shaped overlying zone along the perimeter of the longwall panel is identified for optimal methane drainage during mining. A practical method that helps define the geometry and boundary of this zone is proposed. This study provides a new methodology and a set of engineering principles for the design of optimal co-extraction of coal and methane.

13/00651 Stability of the parting between coal pillar workings in level contiguous seams during depillaring

Singh, R. *et al. International Journal of Rock Mechanics and Mining Sciences*, 2012, 55, 1–14.

In India, there are a number of cases of parting failures in mines due to instability of the parting between contiguous seam workings. So far, no suitable norm exists for predicting the stability of the parting during simultaneous depillaring of contiguous seams or sections, the latter being in thick seams. The factors affecting parting stability in contiguous depillaring have been identified as horizontal to vertical *in situ* stress ratio, width of splits/slices; rock mass rating, parting thickness and combination of different face positions in upper and lower workings. A large number of two- and three-dimensional models were run covering all these variables to arrive at suitable predictive equations to define parting stability and support requirements in contiguous seams/sections during depillaring operations in Indian coal fields. Finally, two representative case studies, briefly discussed in this paper, validated the developed equations for parting stability and support requirements at mine sites.

13/00652 The propagation speed of the cracks in coal body containing gas

Li, X. *et al. Safety Science*, 2012, 50, (4), 914–917.

The destabilization of coal body containing gas that is caused by the quick propagation of the cracks in coal body containing gas and the high pressure gas, which result into coal and gas outburst. Thus, according to the theory of brittleness rupture mechanics the propagation speed calculation formula of the cracks in coal body containing gas is derived under constant stress and the mechanism of the cracks propagation is analysed. The propagation speed of the cracks in coal body containing gas is calculated by the experimental work. The research results show that gas pressure make the cracks propagation easier, which is consistent with the analysis result of the propagation speed calculation of the cracks. As well as the propagation speed of the cracks increase with the augment of gas pressure.

Transport, storage

13/00653 Flow characteristics and stability of dense-phase pneumatic conveying of pulverized coal under high pressure

Cai, L. *et al. Experimental Thermal and Fluid Science*, 2012, 41, 149–157.

Conveying characteristics and flow stability are very important for the design and control of conveying systems under high pressure. The influences of operating parameters (fluidizing gas flow rate and supplementary gas flow rate) and material properties (coal category, particle size and moisture content) on conveying characteristics were investigated in an experimental test facility with the conveying pressure up to 4 MPa. Wavelet transform and Shannon entropy analysis were applied to analysing pressure drops through horizontal pipe in order to obtain stability criterion. Results indicated that with the increase in fluidizing gas flow rate, the mass flow rate of pulverized coal increased at first and then decreased while solid–gas ratio decreased all the way. Conveying phase diagrams and pressure drops through different test sections of pulverized coal under high pressure were obtained and analysed. Conveying optimal moisture content and extreme moisture content were revealed for different coal categories. The influences of coal category and particle size on conveying characteristics were achieved. Through analysing the relationship between Shannon entropy and conveying stability at different operating parameters and material properties, a new method for distinguishing conveying stability was established.

13/00654 Prediction of the height of destressed zone above the mined panel roof in longwall coal mining

Majdi, A. *et al. International Journal of Coal Geology*, 2012, 98, 62–72.

Longwall mining is one of the most widely used underground mining methods most suitable in relatively flat-lying, thick, and uniform coalbeds. Due to extraction of the coal seam, the panel roof strata above the mined zone will be destressed and then the roof loads will be redistributed and transferred to the front abutment and neighbouring solid sections with higher load bearing capacity where the adjacent access tunnels and the corresponding barrier pillars are located. The height of destressed zone (HDZ), in this paper is taken as equivalent to the combined height of the caving and fracturing zones above the mined panel roof induced due to longwall mining. The height of destressed zone plays a vital role in accurate determination of the amount of loads being transferred towards front abutment and panel sides. The paper describes the mechanism of development of the height of this zone. Finally, five new simple, yet conclusive, mathematical approaches to estimate the height of destressed zone are presented. The results of the methods proposed are compared with each other and with the comparable methods. The methods proposed are further compared and verified with *in situ* measurements reported in the literatures. The comparative results confirm the agreement that exist among the methods and those with the *in situ* measurements as well. Finally the methods have shown that, in short term, the height of destressed zone ranges from 6.5 to 24 times the extraction coal seam height; while, in long term, the height of destressed zone ranges from 11.5 to 46.5 times the extraction coal seam height. Therefore, beyond this height the overburden pressure will be transferred towards the front abutment, the adjacent access tunnels, the intervening barrier pillars as well as the panel rib-sides.

13/00655 The caving and sliding control of surrounding rocks on large coal roadways affected by abutment pressure

Li, J. *et al. Safety Science*, 2012, 50, (4), 773–777.

For the caving and sliding control of roadways with large cross-section, thick mudstone roof and abutment pressure influence, the cable truss system is proposed and its support mechanism is thoroughly analysed in this paper. Furthermore, according to the geometric size and ground pressure conditions on field coal roadways Nos. 101, 102 and 103 in Xinyuan coal mine, three types of cable truss support systems are designed for obtaining the optimum cable truss support system. Then the corresponding parameters for each support design are determined by use of the numerical simulation method, and three kinds of support systems are put into practice. The field observation results show that roof should be effectively controlled by the normal cable truss structure consisting of two long cables and one connector, and both coal sides can be protected by the simplified cable truss structure composed of two short cables and one channel bar. Finally, the optimal support system is gotten which is much better than the other two support designs in rock deformation control effect and economic profits.

Economics, business, marketing, policy

13/00656 A graphical CO_2 emission treatment intensity assessment for energy and economic analyses of integrated decarbonised production systems

Ng, K. S. *et al. Computers & Chemical Engineering*, 2012, 45, 1–14.

Design of clean energy systems is highly complex due to the existence of a variety of CO_2 abatement and integration options. In this study, an effective decision-making methodology has been developed for facilitating the selection of lowest energy or lowest cost intensity systems, from a portfolio of flowsheet configurations with different decarbonization strategies. The fundamental aspect of the proposed methodology lies in thermodynamic feasibility assessment as well as quantification of CO_2 emission treatment intensity using a graphical approach (CO_2 emission balance diagram) for energy and economic performance analyses of integrated decarbonized systems. The relationship between the graphical representation and performances is established using blocks and boundaries on integrated systems. The effectiveness of the methodology has been demonstrated through a range of coal gasification-based polygeneration and cogeneration systems, incorporating either of carbon capture and storage or CO_2 reuse options.

13/00657 Assessment of roof fall risk during retreat mining in room and pillar coal mines

Ghasemi, E. *et al. International Journal of Rock Mechanics and Mining Sciences*, 2012, 54, 80–89.

One of the most challenging safety problems in room and pillar coal mines is roof fall phenomena during retreat mining. Roof fall not only causes fatal and non-fatal injuries on miners, stoppages in mining operations and equipment breakdowns, but also results in inefficient recovery of ore reserves. As a result, development of a methodology for risk assessment of roof fall has a remarkable role on safety of retreat mining. In this paper, at first all effective parameters on roof fall during retreat mining are identified and then the role of each parameter on roof fall occurrence is explained. Afterwards, a practical methodology is developed for assessment and control of roof fall risk using semi-quantitative techniques. Finally, this methodology is applied in main panel of Tabas central mine, located in the mid-eastern of Iran, and various possible scenarios of retreat mining and corresponding risks are evaluated.

13/00658 Feasibility of using ash-free coal in a solid-oxide-electrolyte direct carbon fuel cell

Kim, J. P. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11401–11408.

The feasibility of using ash-free coal as the fuel in a direct carbon fuel cell (DCFC) was investigated. Tubular-electrolyte-supported single cells were operated at high temperatures with continuous fuel feeding equipment. A single cell consisted of an yttria-stabilized zirconia (YSZ) electrolyte tube support, a NiO-YSZ cermet anode, and an LSM-YSZ composite cathode. The solvent extraction method was used to remove mineral matter and ash from raw coal. From thermal gravimetric analysis, the ash content of the ash-free coal was found to be nearly zero, but its volatile matter content was 38.34 wt%. Scanning electron microscopy observations and visualization tests were carried out for characterization of the interface of the ash-free coal; the results showed that the ash-free coal was in a liquid-like phase at high temperatures because the volatile matter in the coal produced by solvent extraction could help maintain carbon in the liquid-like state on the anode at high temperatures. The cell performance was affected by this liquid-like state at high temperatures.

13/00659 Risk management and workers' safety behavior control in coal mine

Cao, Q. *et al. Safety Science*, 2012, 50, (4), 909–913.

According to the risk management characteristics and the actual needs of safety production in coal mines, the authors analyse the system of risk management methods in a coal mine and implement it in the Geting coal mine. The system manages and controls the potential accident risks, hazard sources and human behaviour risks. On this basis, the system of workers' safety behaviour control technology in a coal mine is further studied, the 'three disobeying' is classified and managed, the 'three disobeying' database and safety countermeasures database are established, and the application software – the system of risk management and safety countermeasures optimization in coal mine based on B/S mode is developed and applied, which uses intranet to analyse and supervise the 'three disobeying' database, publish early-warning information, optimize management and control countermeasures; at the same time, the important prompting messages can be automatically sent to the mobile phones of relevant managers and the person in charge through public communication system in order to improve the real-time capability and effectiveness of unsafe behaviour control. The technological system and application software implemented in the Geting coal mine has achieved good results.

13/00660 Simulation analysis on structure safety of coal mine mobile refuge chamber under explosion load

Zhao, H. *et al. Safety Science*, 2012, 50, (4), 674–678.

In order to check structural strength of coal mine mobiles refuge chamber, and do security evaluation of the mobile refuge chamber, a refuge chamber model was established, then a finite element method was instituted for it to ensure the refuge chamber would not be severely damaged when gas or coal dust explosion suddenly happened. A triangle shock wave with 1.2 MPa over-pressure, 300 ms lasting time was settled. Explicit non-linear dynamic analysis program was used to simulate response of the refuge chamber. The maximum stress was 244 MPa, located in central part of sides and tail end of the last capsule.

The maximum displacement was 29.32 mm, located in central part of sides and tail end of the last capsule. The calculation indicated that the refuge chamber was not obviously damaged. It could reliable work to meet safety requirements. Compared with the reported experimental results, the simulation method was verified. Based on analysis, suggestions were put forward for further improving.

13/00661 Status and future tasks of coal mining safety in China

He, X. and Li, S. *Safety Science*, 2012, 50, (4), 894–898.

In general, contexts of coal mining safety involve technology, administration and socioeconomic environment as well. This paper presents statistical analysis of Chinese coal mine accidents in recent years and analyses the reasons for the high risk in coal mining from technical and socioeconomic viewpoints. Social and economic reform has been unleashing social, economic factors that are driving a fundamental transformation of new workplace safety problems and making coal mining safety in China take on Chinese features. Compared with major state-owned and local state-owned coalmines, township and village coal mines are most dangerous coal mines with highest occupational risks. The incidence and death toll of ceiling accidents are higher than those of accidents such as gas, machinery, electricity, transportation, flood, and fire. New organizational risks appeared with rapid development of state-owned coal mines' reorganization. Low-skilled labour restricts both technical renovation and safety management. The government has adopted a systematic arrangement to improve coal mining safety such as closing the township and village coalmines that cannot meet the standard of safety, reinforcing the supervision over coal mining safety, strengthening technological renovation and enhancing work safety input.

13/00662 Utility optimization strategy of safety management capability of coal mine – a case study of JCIA

Liu, T.-z. *et al. Safety Science*, 2012, 50, (4), 684–688.

This article describes optimization strategy of safety management capability of coal mines (SMCCM) from the perspective of utility of coal miner with the method of empirical research. Four elements of SMCCM are put forward which consist of 'employee safety knowledge', 'equipment safety knowledge', 'environment safety knowledge' and 'rule safety knowledge'. Eight elements of utility are put forward which consist of 'benefit satisfaction', 'promotion satisfaction', 'job satisfaction', 'enterprise satisfaction', 'management satisfaction', 'colleague satisfaction', 'relationship satisfaction' and 'communication satisfaction'. Then hypotheses of influence path between SMCCM and utility are proposed. Jilin Coal Industry Association (JCIA) is chosen as the sample to carry out survey, which questionnaire is designed based on the Likert six-point scale to avoid the middle tendency of the test samples. Data analysis is done from following angles: analysis of the structure and utility of test samples, variables analysis of SMCCM and utility, model analysis of interaction between SMCCM and utility. And then results are obtained from the analysis of elements of SMCCM and elements of utility. Conclusions: first, 'rule safety knowledge' should be strengthened above all; second, 'job satisfaction' should be paid more attention to; third, coal miner's benefit should be concerned specially.

Derived solid fuels

13/00663 Impact of a semi-industrial coke processing plant in the surrounding surface soil: part I: trace element content

Díaz-Somoano, M. *et al. Fuel Processing Technology*, 2012, 102, 35–45.

Soil pollution by anthropogenic activities is an important environmental issue especially in industrialized countries. The objective of this study is to evaluate the environmental impact of a coal conversion plant on the surrounding soil by measuring the spatial distribution of particulate organic carbon and determining the concentration of trace elements (part I) and PAHs (part II). The results indicate that the surface soil presents an increase in the content of organic particulates with values exceeding 80% vol. at the centre of the coking plant facilities. The concentrations rapidly decrease as the distance from the plant increases. Although concentrations of As, Cd, Co, Cr, Cu, Hg, Ni, Pb and Zn in most cases did not exceed the environmental limits, a clear relationship was established between the presence of some of these elements and the high values of particulate organic carbon content found in the proximity of the plant.

13/00664 Influence of added potassium and sodium carbonates on CO_2 reactivity of the char from a demineralized inertinite rich bituminous coal

Klopper, L. *et al. Journal of Analytical and Applied Pyrolysis*, 2012, 96, 188–195.

The addition of K_2CO_3, Na_2CO_3 and a mixture of the two catalysts showed an increase in the CO_2 reactivity of the char prepared from the demineralized inertinite rich bituminous coal at 900 °C in nitrogen. The CO_2 reactivity of the char is higher when the catalysts are added to the coal before preparing the char in comparison to addition of the catalyst to the prepared char. The distribution of the catalyst on the char particles thus seems to be better upon addition of the catalyst to the coal (before charring). An added effect could be the evolution of CO_2 during charring that may increase the surface area of the produced char. The surface area values of the chars ($>400\,m^2/g$) were higher than the values for the demineralized coal samples (approximately $150\,m^2/g$) and the values for the char prepared from the coal with added catalysts increased from 413 to $445\,m^2/g$. XRF, XRD and QEMSCAN analyses were performed to determine the species of K_2CO_3 and Na_2CO_3 formed during thermal treatment of the samples. KCl, NaCl, K_2O and Na_2O are some of the species that were detected.

13/00665 Large-scale synthesis of multi-walled carbon nanotubes in a continuous inclined mobile-bed rotating reactor by the catalytic chemical vapour deposition process using methane as carbon source

Douven, S. *et al. Chemical Engineering Journal*, 2012, 188, 113–125.

Multi-walled carbon nanotubes (CNTs) were produced in a continuous inclined mobile-bed rotating reactor by the catalytic chemical vapour deposition of methane on a bimetallic Ni–Mo/MgO catalyst whose activity remains constant in the course of time. Measurements performed on the continuous reactor were validated to ensure that the installation worked correctly and that measurements were precise enough. The performance of the reactor was simulated using a model based on the chemical reactor engineering approach. Hypotheses of the model were verified, and a kinetic study was performed to obtain a kinetic rate expression and to determine the catalytic activity as a function of time. The purity level of produced CNTs depends on the desired properties of the product, so the operating conditions are linked to the purity level that is required. A minimal purity level corresponds to high carbon production, and a maximal purity level corresponds to high specific productivity. It was shown that operating conditions had to be fixed to reach a given specific productivity or a given carbon production, and the optimized operating conditions leading to those two opposite purity level objectives were established.

13/00666 Production of char from vacuum pyrolysis of South-African sugar cane bagasse and its characterization as activated carbon and biochar

Carrier, M. *et al. Journal of Analytical and Applied Pyrolysis*, 2012, 96, 24–32.

The potential of vacuum pyrolysis to convert sugar cane bagasse into char materials for wastewater treatment and soil amendment is the focus of this research paper. Vacuum pyrolysis produces both bio-oil and char in similar quantities. Vacuum pyrolysis has the potential to produce high quality chars for wastewater treatment and soil amendment directly during the conversion process, with no further upgrading required. In the present study, chars with the required porous structure was obtained directly from the vacuum pyrolysis process, making it very efficient as adsorbent both in terms of methylene blue (MB) adsorption with a N_2-BET surface area of $418\,m^2\,g^{-1}$. Further steam activation of the chars benefited the development of meso- and macroporosity, although this upgrading step was not essential to achieve the required performance of char as an MB adsorbent. The development of large pores during the vacuum pyrolysis favoured physisorption of MB, rather than chemisorption. The chemical nature of the vacuum pyrolysis char resulted in a slightly acidic surface (pH 6.56). The biochar from vacuum pyrolysis can be considered as a highly beneficial soil amendment, as it would enhance soil nutrient and water holding capacity, due to its high cation exchange capacity ($122\,cmol_c\,kg^{-1}$) and high surface area. It is also a good source of beneficial plant macronutrients and micronutrients and contains negligible levels of toxic elements.

13/00667 Properties and CO_2 reactivity of the inert and reactive maceral-derived components in cokes

Grigore, M. *et al. International Journal of Coal Geology*, 2012, 98, 1–9.

The response of coke to gasification affects its degradation in the blast furnace. Coke gasification with carbon dioxide at high temperature is selective, with the inert maceral-derived component reacting more readily than the reactive maceral-derived component. Previous reactivity studies on carbonized vitrinite- and inertinite-rich fractions indicated that the amount of catalytic mineral phases control their reactivity. However, total Fe, Ca, K and Na from the ash chemistry were used as indicators of the abundance of catalytic material rather than the concentration of the catalytic mineral phases. Additionally, there is disagreement regarding the influence of micropore surface area and average carbon crystallite size on reactivity of the inert maceral-derived component and reactive maceral-derived component. Here the authors examine the influence of the abundance of the catalytic mineral phases on the reactivity of the inert maceral-derived component and reactive maceral-derived component, and also the influences of micropore surface area and average carbon crystallite size. Cokes from inertinite- and vitrinite-rich fractions prepared from four Australian bituminous coals were reacted with carbon dioxide at temperatures between 855 and 934 °C. The major factors that make inert maceral-derived component more reactive than reactive maceral-derived component at the initial stages were found to be the concentration of catalytic mineral phases and micropore surface area. The catalytic mineral phases identified in the coked inertinite- and vitrinite-rich fractions were metallic iron, pyrrhotite, troilite, wustite, magnetite and hematite. No Ca, K and Na catalytic mineral phases were identified in any of the studied cokes. The average crystallite height was not found to be a major factor controlling coke reactivity at the initial stages.

13/00668 The effects of hydrogen on KOH activation of petroleum coke

Xiao, R. *et al. Journal of Analytical and Applied Pyrolysis*, 2012, 96, 120–125.

KOH activation of petroleum coke (PC) was conducted with 30 vol% H_2 + 70 vol% N_2 as carrier gas. TG-DTG, FTIR, elemental analysis, N_2 adsorption, GC and XRD techniques were used to investigate the effects of hydrogen on the activation. During the initial stage of the activation, i.e. the carbonization of the PC, additional –CH– and –CH_2– species were formed due to the chemisorption of hydrogen on the nascent sites of the PC created by the removal of the surface heteroatom groups. The formation of the –CH– and –CH_2– species increased the quantity of 'active sites' which is favourable to the further activation reaction, and developed the porous structure of the activated carbons. The micropore volume and BET surface areas of the activated carbon prepared under 30 vol% H_2 + 70 vol% N_2 and with a relatively low KOH/PC weight ratio of 2:1 have been increased from 0.78 cm^3/g and 1936 m^2/g to 0.97 cm^3/g and 2477 m^2/g, respectively, compared to that prepared in pure N_2 atmosphere with the same KOH/PC ratio.

02 LIQUID FUELS

Sources, properties, recovery

13/00669 A method for aquifer identification in petroleum reservoirs: a case study of Puerto Ceiba oilfield

Cosultchi, A. *et al. Journal of Petroleum Science and Engineering*, 2012, 94–95, 55–65.

The paper describes an efficient multi-stage data-driven method for aquifer and water influx pattern classification. It is based on statistical multivariate analysis techniques, principal components analysis and cluster analysis. The main advantage of the proposed method is the integration of the analysis of static (water and oil properties) and dynamic (production series) data in order to understand the water-related behaviour of the oilfield. For oilfield aquifers classification, oil and water physicochemical properties are used. Water influx pattern classification consists of three steps. Firstly, single-well production data analysis techniques are applied: (1) conventional decline curve analysis; and (2) a novel water-cut curve analysis with a logistic growth equation. Secondly, the obtained parameters are employed for the statistical multivariate analysis of the field. Finally, logistic-type equation parameters are used for qualitative identification of velocity of water entrance, water amount and first date of water entrance. The proposed method is discussed and illustrated using Puerto Ceiba case study. The work is a step forward towards the introduction of data-driven approaches in the engineering practices of water control.

13/00670 CFD modeling of the effect of polymer elasticity on residual oil saturation at the pore-scale

Afsharpoor, A. *et al. Journal of Petroleum Science and Engineering*, 2012, 94–95, 79–88.

Polymers are used in enhanced oil recovery (EOR) to increase sweep efficiency, but recent experimental and field data suggest that viscoelastic polymers such as hydrolysed polyacrylamide (HPAM) reduce residual oil saturation as well. The observed reduction contradicts decades of belief that polymers could not be used to reduce residual oil because the additional pressure required to overcome capillary pressure is orders of magnitude greater than provided by the more viscous polymer. However, additional forces (such as normal stress forces) may be significant for viscoelastic fluids that are ignored in analysis of purely viscous fluids. The authors perform computational fluid dynamics (CFDs) simulations of viscoelastic flow around static oil droplets in geometries representative of pore throats. They show that normal forces are significant for viscoelastic fluids and increase with *De* and the total force imposed on the droplet may be larger than an equivalent Newtonian fluid with the same viscosity. Results indicate that normal forces could dominate and the total, effective force would be enough to mobilize trapped oil.

13/00671 Detailed compositional analysis of hydrocarbons in soil gases above multi-horizon petroleum deposits – a case study from western Poland

Sechman, H. *Applied Geochemistry*, 2012, 27, (10), 2130–2147.

A surface geochemical survey was carried on in an area with a cluster of petroleum deposits in western Poland. The largest of these accumulations is the Paproć-Cicha Góra dry gas deposit reservoired in the Rotliegend sediments. Other, similar gas deposits are: the Paproć gas field discovered in the top part of the Carboniferous formation and the Paproć W, Paproć N, and Nowy Tomyśl gas fields localized in the Zechstein Limestone reef structures. Moreover, the Paproć gas-condensate and the Jastrzębsko oil deposits were found at shallower depths, in the Main Dolomite formation. This paper aims to analyse the variability of composition and distribution of near-surface gaseous hydrocarbons in relation to hydrocarbon accumulations reservoired in various stratigraphic units at depths. The occurrence of CH_4, its heavier homologues and unsaturated hydrocarbons was measured in 267 soil gas samples. The sampling sites were located along six survey lines (A–A, B–B, C–C, D–D, E–E and F–F) at a 200 m spacing. Concentrations of CH_4, total alkanes (C_2–C_4) and total alkenes (C_2–C_3) reached maxima of 0.26 vol.%, 5.32 ppm and 5.88 ppm, respectively. Soil–gas alkanes heavier than CH_4 were interpreted as being derived from subsurface hydrocarbon accumulations. These compounds penetrated to the near-surface zone by means of active and passive microseepage. Source strength of alkanes microseepage from subsurface accumulations to the land surface (determined by the C_2H_6/C_2H_4 ratio) is not a factor that substantially changes the patterns of surface anomalies. Analysis of the values of CH_4/C_2H_6 and C_2H_6/C_3H_8 coefficients confirmed the presence of compositionally diversified, deep hydrocarbon accumulations. The study revealed that even small accumulations of gas condensate produce very strong surface geochemical signatures, contrasting with dry gas deposits. The reason may be a specific effect of hydrocarbon migration within the existing petroleum system. The Main Dolomite, which is both the source and the reservoir rock in the Fore-sudetic monocline, plays the role of a 'filter', which modifies the flux of gases ascending from deep-seated reservoirs. As a result of such 'filtering', the geochemical signature of hydrocarbons recorded at the surface indicates the dominance of gas condensate and oil–gas accumulations at depths, giving rise to obviously incorrect interpretations. These interpretations were evidenced by compositional analysis of soil gases, which did not explicitly confirm the existence of a dry gas deposit in the Rotliegend reservoir (Paproć-Cicha Góra gas field). On the other hand, the identified anomalies generally reflect the outline of this accumulation. It supports the applicability of surface geochemical surveys to hydrocarbon exploration in the Fore-sudetic Monocline. The presence of the Main Dolomite at shallower depth must be taken into account in the interpretation of data used for positioning of seismically identified Rotliegend structures. The results of this project indicate that the Main Dolomite may obscure the geochemical signature of near-surface gases derived from dry gas accumulations in both the deeper Rotliegend and Carboniferous reservoirs.

13/00672 Determination of specific gravity and kinematic viscosity of diesel using distillation curves and multivariate calibration

Aleme, H. G. *et al. Fuel Processing Technology*, 2012, 102, 90–95.

In order to predict specific gravity and kinematic viscosity, distillation curves (used in the quality control of diesel) were associated with the partial least squares method (PLS). The regression coefficients of the algorithms were compared after selecting the appropriate number of latent variables for each prediction. The low values (0.82 kg m^{-3} and 0.095 $mm^2\,s^{-1}$) obtained for root mean squared error prediction and the high correlation coefficients (0.9973 and 0.9943) between real and predicted values showed that PLS associated with distillation curves was efficient to determine specific gravity and kinematic viscosity. Models created with diesel samples of different composition were used for these predictions, thus reflecting the variety of fuel in the Brazilian market. In addition, the proposed method is low cost and easy to carry out, since it resorts to the results of a routine assay performed to assess the quality of highway diesel fuel.

13/00673 Estimation of crude oil TBP from crude viscosity

Argirov, G. *et al. Fuel*, 2012, 97, 358–365.

Crude oil true boiling point (TBP) curves are well recognized as an important characteristic, needed to determine the potential of fractions obtained by distillation, to monitor distillation units, to verify the identity of crude oil samples, etc. They can be obtained experimentally or calculated by a variety of methods, which have different precision. The precision of the particular method determines the applicability of the obtained TBP data. Riazi's two-parameter distribution model and experimental crude assay data for 117 crudes from all over the world have been used to derive a model for prediction of TBP curves from the kinematic viscosity of the samples at 37.8 °C. The model was tested by prediction of the cumulative mass fractions of all studied crude samples. It was found that the TBP distribution for fractions boiling up to 340 °C could be predicted with an average relative deviation of the order of 5.95%. This is higher than the respective deviation of previously proposed models, e.g. Riazi's model, with an average deviation of 3.3%. Due to that reason the model was improved for prediction of light crude TBP curves. It results to falling down of the average relative deviation to 3.74%. However, these models require experimental data for several properties, while in practical terms the precision of this model is sufficient to detect any significant upsets in the operation of refinery crude distillation units (CDUs), so its computerized procedure may be used as a quick tool for monitoring of the CDU operation.

13/00674 Heat transfer characteristics during subcooled flow boiling of a kerosene kind hydrocarbon fuel in a 1 mm diameter channel

Liu, Z. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (19–20), 4987–4995.

The subcooled flow boiling heat transfer characteristics of a kerosene kind hydrocarbon fuel were investigated in an electrically heated horizontal tube with an inner diameter of 1.0 mm, in the range of heat flux: 20–1500 kW/m^2, fluid temperature: 25–400 °C, mass flux: 1260–2160 kg/m^2 s, and pressure: 0.25–2.5 MPa. It was proposed that nucleate boiling heat transfer mechanism is dominant, as the heat transfer performance is dependent on heat flux imposed on the channel, rather than the fuel flow rate. It was found that the wall temperatures along the test section kept constant during the fully developed subcooled boiling (FDSB) of the non-azeotropic hydrocarbon fuel. After the onset of nucleate boiling, the temperature differences between inner wall and bulk fluid begin to decrease with the increase of heat flux. Experimental results show that the complicated boiling heat transfer behaviour of hydrocarbon fuel is profoundly affected by the pressure and heat flux, especially by fuel subcooling. A correlation of heat transfer coefficients varying with heat fluxes and fuel subcooling was curve fitted. Excellent agreement is obtained between the predicted values and the experimental data.

13/00675 Laboratory characterisation of shale properties

Josh, M. *et al. Journal of Petroleum Science and Engineering*, 2012, 88–89, 107–124.

Shale gas has become a significant resource in the USA over the past few years and companies are now evaluating the shale gas potential of many sedimentary basins, including several onshore basins within Australia. The renewed focus on rock sequences that have hitherto largely been ignored has necessitated the development of workflows and methods for characterizing shales. Laboratory characterization of rock properties is an important part of any resource evaluation and for shale gas, specific properties of importance include silt content, organic matter abundance and type, static and dynamic mechanical properties (brittleness), micro/macro-fabrics, porosity, permeability, petrophysical properties and anisotropy. Here a workflow is introduced for systematic shale characterization in the laboratory with a number of examples to illustrate and discuss the application to reservoir evaluation in shale gas plays. A suite of shales from a number of sedimentary basins around the world was collected and characterized with a full suite of non-destructive petrophysical methods before destructive geomechanical testing was performed. For each sample, a representative portion was analysed for quantitative mineralogy using XRD and XRF, and clay chemical reactivity via cation exchange capacity (CEC) and grain size by centrifugation. For many samples, surface area and mercury injection capillary pressure (MICP) for porosity and pore throat distribution were also performed and used to predict permeability from models available in the literature. Several imaging techniques including scanning electron microscopy (SEM) and X-ray computed (micro-)tomography (X-ray CT) at low and high resolution were performed. Shale strength has previously been shown to be related to CEC, which is inversely proportional to silt content. Anisotropy of shale properties is both intrinsic and stress-induced. Dielectric properties are related to water content at high frequency and dispersion in the dielectric constant is directly related to CEC of clays in particular and hence rock strength. Stress-induced anisotropy of elastic properties was found to be dependent on the orientation of microfabrics with respect to the maximum principal stress direction. Low and high field nuclear magnetic resonance can be used to distinguish clay-bound and free water as well as adsorption of organic components and to screen for wettability. High and low field NMR techniques are combined to show that illitic shales tend to be strongly water wet while the presence of kaolinitic clays imparts a tendency for shales to become oil wet with likely consequences for oil/gas recovery strategy, production flow efficiency and drilling design.

13/00676 Markers for secondary reactions of migrated crude oil on carbonaceous surfaces

Alexander, R. *et al. Organic Geochemistry*, 2012, 49, 30–35.

A high abundance of ethyl substituted aromatic hydrocarbons (HCs) relative to their methyl counterparts is an unusual feature of some crude oils. Enhanced stability of ethyl aromatic HCs in the presence of tetralin was observed when individual ethylated compounds were heated with activated carbon in sealed tubes over a range of 170–340 °C. In addition, conversion of the common distribution of alkyl aromatic HCs to an unusual distribution, containing a higher relative abundance of ethyl compounds, was demonstrated by way of closed system heating of the aromatic fraction of a crude oil in the presence of activated carbon. The conditions for this unusual process require the presence of hydrogen donor components, which selectively limit the reaction and depletion of ethylated compounds relative to methylated compounds. The phenomenon has been shown to occur for substituted benzenes, naphthalenes, phenanthrenes and biphenyls. Enhanced abundance of ethyl aromatic HCs relative to their methylated counterparts is therefore proposed as an indicator for secondary reactions of migrated crude oil that has undergone thermal alteration after contact with carbonaceous surfaces in sediments. Application of these principles to selected crude oils and sediment extracts from the Carnarvon and Cooper/Eromanga Basins (Australia) indicates that significant secondary reaction of migrated crude oil has occurred.

13/00677 Origin of the unusually high dibenzothiophene oils in Tazhong-4 oilfield of Tarim Basin and its implication in deep petroleum exploration

Li, S. *et al. Organic Geochemistry*, 2012, 48, 56–80.

Unusually high dibenzothiophene (DBT) concentrations are present in the oils from the Tazhong-4 oilfield in the Tazhong Uplift, Tarim Basin. Positive-ion electrospray ionization Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) was used in combination with conventional geochemical approaches to unravel the enrichment mechanisms. Significant amounts of S_1 species with relatively low DBE values (0–8), i.e. sulfur ethers, mercaptans, thiophenes and benzothiophenes, were detected in three Lower Ordovician oils with high thermal maturity, which were suggested to be the products of thermochemical sulfate reduction (TSR) in the reservoir. The occurrence of TSR was also supported by the coexistence of thiadiamondoids and abundant H_2S in the gases associated with the oils. Obviously low concentrations of the DBE = 9 S_1 species (mainly equivalent to C_0–C_{35} DBTs) compared to its homologues were observed for the three oils which were probably altered by TSR, indicating that no positive relationship existed between TSR and DBTs in this study. The sulfur compounds in the Tazhong-4 oils are quite similar to those in the majority of Lower Ordovician oils characterized by high concentrations of DBTs and dominant DBE = 9 S_1 species with only small amounts of sulfur compounds with low thermal stability (DBE = 0–8), suggesting only a small proportion of sulfur compounds were derived from TSR. It is thermal maturity rather than TSR that has caused the unusually high DBT concentrations in most of the Lower Ordovician oils. The authors suggest that the unusually high DBT oils in the Tazhong-4 oilfield are caused by oil mixing from the later charged Lower Ordovician (or perhaps even deeper), with high DBT abundances from the earlier less mature oils, which was supported by the oil mixing experiments and previous relevant investigations as well as abundant authigenic pyrite of hydrothermal origin. The authors believe that TSR should have occurred in the Tazhong Uplift based on the FT-ICR MS results. However, normal sulfur compounds were detected in most oils and no increase of $\delta^{13}C_2H_6$–$\delta^{13}C_4H_{10}$ was observed for the gas hydrocarbons, suggesting only a slight alteration of the oils by TSR currently and/or recently. The authors suspect that the abnormal sulfur compounds in the Lower Ordovician oils might also be a result of deep oil mixing, which might imply a deeper petroliferous horizon, i.e. Cambrian, with a high petroleum potential. This study is important to further deep petroleum exploration in the area.

13/00678 Oxy-fuel combustion: the effect of coal rank and the role of char-CO_2 reaction

Dhaneswar, S. R. and Pisupati, S. V. *Fuel Processing Technology*, 2012, 102, 156–165.

The role of coal rank during oxy-fuel (O_2/CO_2) combustion is investigated using a suite of four coals. Combustion tests carried out in a drop-tube reactor under air and oxy-fuel atmospheres showed that for the lower rank coals, Beulah (lignite) and Dietz (subbituminous coal), oxy-fuel combustion produced a higher carbon conversion compared to air combustion at both short and long residence times. For Pittsburgh (high volatile) coal, oxy-fuel combustion produced a higher carbon conversion compared to air combustion only at longer residence times. On the other hand, for the Pocahontas coal (highest rank coal used in this study), oxy-fuel combustion produced a lower conversion than air combustion at all residence times. The higher conversion in low-rank coals under oxy-fuel conditions was due to the exponential increase in the char-CO_2 reaction rate occurring at high temperatures (>1500 K). This was shown by theoretical rate extrapolation to high temperatures, using intrinsic rate parameters generated using thermogravimetric analyser (TGA). The char particle temperatures were modelled under oxy-fuel atmospheres and the results showed a significant role of the char-CO_2 reaction at high temperatures and high CO_2 partial pressures. The role of ion-exchangeable cations during oxy-fuel combustion in catalysing the reactions particularly in low rank coals was investigated. Ammonium acetate washed samples indicated a significant reactivity loss in the TGA but the conversion was unaffected in DTR at 1873 K, suggesting that catalytic activity is not significant under practical combustion conditions.

13/00679 Prediction of the SARA analysis of Colombian crude oils using ATR–FTIR spectroscopy and chemometric methods

Meléndez, L. V. *et al. Journal of Petroleum Science and Engineering*, 2012, 90–91, 56–60.

In this work eight chemometrics models to predict saturates, aromatics, resins and asphaltenes (SARA) composition of 50 Colombian crudes oils using Fourier transform infrared coupled to attenuated total reflectance (ATR–FTIR) spectra were developed. The samples were correlated by similarity using principal components analysis (PCA) with their ATR–FTIR spectra. The validation showed satisfactory results for the prediction of the SARA analysis of crude oils. For each SARA component, standard errors of prediction (SEP) for light samples were 1.9, 1.7, 1.3 and 0.4. For heavy samples SEP were 2.5, 1.7, 3.7 and 1.4. In all cases, the coefficients of correlation (R2) between the values of reference and those predicted by the models were superior to 0.95. The IR spectroscopy coupled with the ATR cell plus chemometric techniques provide an alternative way for the quantitative prediction of the weight-percentage SARA group-types with minimal handling of the samples in a short period of time.

13/00680 Quantifying saline groundwater seepage to surface waters in the Athabasca oil sands region

Jasechko, S. *et al. Applied Geochemistry*, 2012, 27, (10), 2068–2076.

Western Canadian oil sands contain over 170 billion barrels of proven unconventional petroleum reserves currently extracted at 1.8 million barrels per day by either surface mining, or by *in situ* techniques that require subsurface injection of steam and hydrocarbon solvents. Natural high-salinity springs are known to add water and entrained inorganic and organic constituents to the Athabasca River and its tributaries in the region of on-going bitumen production. However, the magnitude and synoptic distribution of these saline inputs has remained unquantified. Here, a chloride mass balance is used to estimate saline groundwater discharge to the Athabasca River from 1987 to 2010. Results show that the highest saline water discharge rate to the Athabasca River occurs between Ft. McMurray and the Peace-Athabasca Delta, supported by subcrop exposure of lower Cretaceous- and Devonian-aged formations bearing saline waters. Further, the input of saline groundwater is found to be an important control on the chemistry of the lower Athabasca River, despite comprising 10^{-1} to 3% of the Athabasca River's discharge. The flux of natural saline groundwater entering the Athabasca does not appear to have increased or decreased from 1987 to 2010. The origin of seep salinity is interpreted as relict subglacial meltwater that has dissolved Devonian-aged evaporites, supported by saline Na-Cl type waters with low $^{18}O/^{16}O$ and $^{2}H/^{1}H$ ratios relative to modern precipitation. The magnitude of groundwater discharge and its impact on the Athabasca River's chemistry in the area of on-going bitumen development warrants the incorporation of natural groundwater seepages into surface water quality monitoring networks.

13/00681 The effect of temperature on the molecular structure of Raman asphaltenes during pyrolysis

Akmaz, S. *et al. Journal of Analytical and Applied Pyrolysis*, 2012, 96, 139–145.

Asphaltenes were precipitated from Raman heavy crude oil subjected to pyrolysis at temperatures of 350, 400 and 450 °C for holding times ranging from 10 to 120 min using sandbath. Product fractions were separated as gas, maltene, remaining asphaltene and coke. The time and temperature dependence of product distributions were determined. Molecular structure of remaining asphaltenes was characterized by elemental analysis, proton nuclear magnetic resonance, gel permeation chromatography. These data provide insights into the distribution of heteroatoms and the aromaticity within both original and remaining asphaltenes as well as to the coke formation reactions occurring during the asphaltene pyrolysis. The temporal structural variations of remaining asphaltene allowed discernment of asphaltene thermal pathways.

Transport, refining, quality, storage

13/00682 A conceptual framework to model interfacial contamination in multiproduct petroleum pipelines

Patrachari, A. R. and Johannes, A. H. *International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4613–4620.

Interfacial contamination of batches of refined petroleum products transported through multiproduct pipelines is a long standing problem in the petroleum industry. Determination of the extent of mixing depends on various factors including fluid properties, operating conditions and flow regimes. The convective-diffusion model along with a fictional parameter, known as the axial dispersion coefficient introduced by Sir G. I. Taylor, is the commonly employed methodology to evaluate longitudinal mixing. However, the model was formulated with a uniform turbulent or laminar flow across the entire flow field. It is argued that the assumption of a uniform flow regime leads to inaccuracies in predicting the extent of contamination at the interface. This study incorporates both the turbulent and the viscous effects in predicting the interfacial contamination volume. Taylor's analysis of dispersion coefficients has been reviewed, and an improved model combining the weighted effects of the viscous boundary layer contributions and the turbulent core contributions to axial dispersion is proposed. The proposed model provides a possible explanation for the underlying physics of interfacial contamination in flow through straight pipes without pipe fittings and other devices. A comparison of the model predictions with literature data demonstrates the importance of considering both turbulent and viscous effects to achieve better overall prediction accuracy.

13/00683 A study on optimizing delivering scheduling for a multiproduct pipeline

Yongtu, L. *et al. Computers & Chemical Engineering*, 2012, 44, 127–140.

Multiproduct pipeline is one of the major ways to connect the large refineries and the consumer markets. The primary task of a pipeline operator is to make scheduling plans which can meet the demands of the delivery stations and maintain the normal operations of the pipeline. In this paper, the objective function is to minimize the total deviation of delivering operation time-windows from due time-windows at each station, with the customers' demand to be satisfied maximally within the time limits. A mathematical model of optimizing scheduling plan for each delivery station has been established and an optimal scheduling plan has been worked out through the heuristic rule. Furthermore, based on analyses, a scheduling simulation software for a multiproduct pipeline has been developed and successfully applied to the operation and management of several multiproduct pipelines in China.

13/00684 An improved crude oil atmospheric distillation process for energy integration: part II: new approach for energy saving by use of residual heat

Benali, T. *et al. Applied Thermal Engineering*, 2012, 40, 132–144.

In Part I of this paper, it was shown on thermodynamic grounds that introducing a flash in the preheating train of an atmospheric oil distillation process, together with an appropriate introduction of the resulting vapour into the column, could potentially bring substantial energy savings, by reducing the duty of the preheating furnace, by doing some pre-fractionation and by reducing the column irreversibilities. Part II expands on this idea by showing how this can be done while keeping the throughput and the product characteristics unchanged. The outcome is that placing several flashes after the heat exchangers and feeding the corresponding vapour streams to the appropriate trays of the column reduces the pumparound flows and the heat brought to the preheating train. The resulting heat deficit may then be compensated in an additional heat exchanger by using low-level heat recuperated from the products of the distillation and/or imported from other processes. The use of this residual heat reduces the furnace duty by approximately an equivalent amount. Thus high-level energy (fuel-gas burnt in the furnace) is replaced by residual low level heat. The simulation with an example flowsheet shows that the savings on fuel could be as high as 21%.

13/00685 Effect of transition metal oxides catalysts on oxidative desulfurization of model diesel

Wan Abu Bakar, W. A. *et al. Fuel Processing Technology*, 2012, 101, 78–84.

In this paper, model diesel is used to study the performance of oxidative desulfurization (ODS) system compared to hydrodesulfurization (HDS) process. A detailed parametric experimental study was performed to select the best technique for sulfur removal. The effects of solvent, oxidant, bimetallic oxide catalyst, dopant, dopant ratio and calcination temperature were investigated. Dimethylformamide (DMF) and tert-butyl hydroperoxide (TBHP) were found to be the best solvent and oxidizing agent for the removal of sulfur compounds in model diesel. Both solvent and oxidant were then applied to explore the applicability of various catalysts, such as iron, manganese, molybdenum, tin, zinc and cobalt in model diesel. The results showed that the catalytic activity was decreased in the order: $Mo > Mn > Sn > Fe \approx Co > Zn$. Further investigation of doped molybdenum revealed that 4.35% WO_3/16.52% MoO_3/Al_2O_3 in the ratio of 10:90 with calcination temperature at 500 °C was assigned as the best catalyst in this research. Under mild reaction condition, this catalyst showed high conversion with appreciable stability until 150 hours and can be used as a reusable active catalyst in ODS treatment. Additionally, on the basis results obtained, a mechanistic proposal for this reaction was postulated, as an oxidation mechanism by nucleophilic attack of the sulfur atom on peroxo species of $WO_3/MoO_3/Al_2O_3$.

13/00686 Effects of aromatics on desulfurization of liquid fuel by π-complexation and carbon adsorbents

Wang, L. *et al. Chemical Engineering Science*, 2012, 73, 208–217.

Equilibrium adsorption of thiophenic sulfur compounds, thiophene (T), benzothiophene (BT), and dibenzothiophene (DBT), from their binary solutions in n-octane and ternary solutions in n-octane and benzene, on three sorbents (activated carbon (AC), $AgNO_3$/MCM-41 and Cu(I)–Y) were studied systematically. Fixed-bed adsorption/breakthrough experiments on these sorbents were also carried out. For all thiophenic sulfur compounds in both binary and ternary solutions, the sorbent adsorption capacities followed the order: Cu(I)–Y>$AgNO_3$/MCM-41>AC. For each sorbent, the selectivity of adsorption of thiophenic sulfur compounds from liquid solutions followed the order: DBT>BT>T>benzene. The experimental results were well interpreted by molecular orbital calculation results. For ternary solutions, benzene competed against thiophenic sulfur compounds for adsorption sites, resulting in reduced thiophenic sulfur adsorption on the studied sorbents. Based on the single-solute Langmuir–Freundlich isotherms, the extended Langmuir–Freundlich isotherm (for multi-component equilibrium adsorption) was used to predict adsorption in ternary solutions, which was in fair agreement with the experimental results. The Cu(I)–Y sorbent was fully regenerable.

13/00687 Fatigue crack growth rate of API X70 steel pipelines under spectrum loading

Beden, S. M. *et al. International Journal of Pressure Vessels and Piping*, 2012, 96–97, 7–12.

Pipelines offer the most efficient way to transport bulk quantities of gas and oil, either from points of production to storage locations or from storage locations to distributed points of end use. As one of the main materials of west–east gas transmission pipes, X70 pipelines usually serve under variable amplitude loading (VAL). Base on the importance of in-service API X70 pipelines, it is important for the safe operation of this system to know its behaviour under VAL. This paper focuses on the ability of using the NASGRO model to predict the fatigue crack growth (FCG), based on investigation with the modified Wheeler model and experimental data. The results show that the NASGRO model gives a fatigue life near to that published in the literature and also showed the FCG rate response of X70 pipeline steels when exposed to VAL with different overload values. Extra modification to the NASGRO model may lead to better representing of FCG rate.

13/00688 Improving fuel quality by whole crude oil hydrotreating: a kinetic model for hydrodeasphaltenization in a trickle bed reactor

Jarullah, A. T. *et al. Applied Energy*, 2012, 94, 182–191.

Fossil fuel is still a predominant source of the global energy requirement. Hydrotreating of whole crude oil has the ability to increase the productivity of middle distillate fractions and improve the fuel quality by simultaneously reducing contaminants such as sulfur, nitrogen, vanadium, nickel and asphaltene to the levels required by the regulatory bodies. Hydrotreating is usually carried out in a trickle bed reactor (TBR) where hydrodesulfurization (HDS), hydrodenitrogenation (HDN), hydrodemetallization (HDM) and hydrodeasphaltenization (HDAs) reactions take place simultaneously. To develop a detailed and a validated TBR process model which can be used for design and optimization of the hydrotreating process, it is essential to develop kinetic models for each of these reactions. Most recently, the authors have developed kinetic models for all of these chemical reactions except that of HDAs. In this work, a kinetic model (in terms of kinetic parameters) for the HDAs reaction in the TBR is developed. A three phase TBR process model incorporating the HDAs reactions with unknown kinetic parameters is developed. Also, a series of experiments has been conducted in an isothermal TBR under different operating conditions affecting the removal of asphaltene. The unknown kinetic parameters are then obtained by applying a parameter estimation technique based on minimization of the sum of square errors (SSEs) between the experimental and predicted concentrations of asphaltene compound in the crude oil. The full model with the estimated kinetic parameters is then applied to evaluate the removal of asphaltene (thus affecting fuel quality) under different operating conditions (than those used in experiments).

13/00689 Inferential monitoring and optimization of crude separation units via hybrid models

Mahalec, V. and Sanchez, Y. *Computers & Chemical Engineering*, 2012, 45, 15–26.

The hybrid model of a CDU introduced in this work can be used for both production planning and for RTO, since the model converges rapidly via SLP, it is small in size, its accuracy is comparable to rigorous models, and it can optimize the operating variables, including furnace duty and pumparound duties. This enables CDU part of the planning models to be as accurate as the RTO models, instead of using standard CDU modes of operation. The model includes mass and energy balances and statistical models relating crude distillation curve points, tower operating variables and tray temperatures to product distillation curves. Hybrid model of a sample CDU shows excellent agreement with property predictions from the rigorous model; RMSE of points on the product distillation curves is typically less than 0.5% of the rigorous model predictions. Optimization of the hybrid model via SLP converged to a better point than equation-oriented AspenPlus.

13/00690 Influence of key parameters on crude oil desalting: an experimental and theoretical study

Vafajoo, L. *et al. Journal of Petroleum Science and Engineering*, 2012, 90–91, 107–111.

Desalting plants are often installed in crude oil production units in order to remove water-soluble salts from an oil stream. Experiments in both the laboratory and field have shown the desalting process parameters to be very complicated. This research reflects the results of a study conducted regarding the impact of operational desalting parameters, including the effects of temperature, injected chemicals and the pH of the crude oil associated water, on an electrostatic desalter on one of the oil platforms owned by the Iranian Oil Offshore Company in the Persian Gulf. The temperature range applied was between 98 to 133 °C, at which the effects on water and oil density as well as salt efficiency and basic sediment and water (BS&W) were studied. The results demonstrate that for high desalting efficiency a temperature between 115 to 120 °C is required. In order to determine which demulsifier provides optimum conditions, the functions of various demulsifiers (noted as C, D, E, F, G and H) on a water–oil emulsion were tested in the laboratory, with C and F providing the optimum output. Accordingly, the field test utilized these two selected demulsifiers. Injection of 50–100 ppm demulsifier produced optimum separation of 88% for BS&W and approximately 99% for salt. Furthermore, the effect of pH of the crude oil in the water–oil emulsion samples was tested in the laboratory and a suitable range determined to be between 9 and 12. Theoretical calculations utilizing fuzzy logic were performed. These showed satisfactory agreement between the experimental and theoretical results obtained.

13/00691 Investigation of the oxidative desulfurization of LCO model mixture by GC-MS and FTIR spectroscopy

Toteva, V. *et al. Fuel Processing Technology*, 2012, 101, 101–105.

The present study describes oxidative desulfurization of a model mixture of fluid-catalytic-cracked light cycle oil (LCO). Oxidations of the sulfur compounds have been monitored by FTIR spectroscopy. Oxidized sulfur compounds and degree of desulfurization by oxidation have been determinate by gas chromatography–mass spectroscopy. It has been established that after oxidation and proper extraction process about 90% of the highly refractive by hydrodesulfurization sulfur compound like 4,6-dimethyl-dibenzothiophene is removed from the oxidized model mixture.

13/00692 Modeling the thermo-hydraulic performance of direct fired heaters for crude processing

Morales-Fuentes, A. *et al. Applied Thermal Engineering*, 2012, 39, 157–162.

Although fouling in heat exchangers for crude processing has received much attention in recent years, the problem still remains unsolved and the economic losses associated to it are significant. Development and application of fouling models due to coke deposition on the heat transfer surface have been achieved with a high degree of certainty for situations where single phase occurs. A simple model to predict fouling rates and its effect on the thermohydraulic performance of fired heaters has been introduced in this paper. The prediction is based on the use of a deposition-removal model that can be applied to both single phase and two-phase flow. Solution of the model shows that the region of the fired heater most affected by fouling corresponds to that where single-phase flow occurs. This indicates that fouling rates in this region is dependent on shear stress. Reduction of fouling rates can be achieved by any means whose final result is the increase of the single phase heat transfer coefficients; for instance: stream velocity or the use of mechanical devices that promote turbulence and reduce the wall boundary layer. As fouling builds up, the crude outlet temperature can only be maintained by increased fuel consumption. For instance, fuel consumption doubles after 9 months of operation. This situation results in higher operating costs plus the corresponding carbon dioxide increase due to the combustion of larger amounts of fuel. However, this is not the only detrimental effect of fouling; since the deposition of coke on the heat transfer surfaces creates a pressure drop rise which reaches its peak when the flow system is no longer capable of maintaining the crude flow rate leading to production losses. Little information on plant data for fired heaters is available in the open literature; future work along this line requires the validation of the proposed fouling models and their improvement.

13/00693 Olefin/paraffin separation using membrane based facilitated transport/chemical absorption techniques

Faiz, R. and Li, K. *Chemical Engineering Science*, 2012, 73, 261–284.

Seeking alternative olefin/paraffin separation techniques have been attracting great interest due to the high operating and capital costs of current commercially practiced separation processes. An olefin/paraffin separation scheme using membrane-based facilitated transport/chemical absorption techniques offers great advantages such as reducing the operating and capital costs, as well as eliminating the operating drawbacks occurring in absorption processes such as flooding, foam formation, etc. Consequently, the utilization of a facilitated transport/chemical absorption scheme with a suitable membrane system for olefin/paraffin separation would be an attractive option for the replacement of the current separation technologies. A comprehensive review is presented for application of membranes for light olefin/paraffin separation. This article covers all types of membrane based facilitated transport/chemical absorption techniques which include various conventional liquid membranes configurations, membrane contactors and more advanced solid membrane electrolytes. The performance evaluation, shortcomings, and advantages are discussed in details.

13/00694 Structural reliability of offshore platforms considering fatigue damage and different failure scenarios

Gholizad, A. *et al. Ocean Engineering*, 2012, 46, 1–8.

Structural systems will normally fail as a consequence of a chain of different components failures. In this paper, fatigue reliability of fixed offshore platforms is investigated by analysing different failure scenarios. In order to evaluate the occurrence probability of a special scenario, it is divided into a finite number of sub-scenarios. All combinations of time sequences are generated for a given sequence of failures, using a specially developed program. In order to calculate the occurrence probability of each scenario, a massive reliability analysis should be done for each of corresponding sub-scenarios. A large number of sub-scenarios should be analysed, therefore implementing time consuming traditional methods for evaluating fatigue reliability may be unrealistic, and a simplified and accurate method is required. Herein, an 'artificial transfer function' is used to calculate the cumulative fatigue degradation in components. The preciseness of the proposed method is evaluated using a numerical model, and then, it is used to calculate the occurrence probability of each sub-scenario. Based on the calculated values, probability of occurrence is obtained for each scenario, and finally, the failure probability of entire system is calculated. The proposed method can be used in inspection planning and evaluating the life extension of existing offshore platforms.

Economics, business, marketing, policy

13/00695 A comparative study of continuous-time models for scheduling of crude oil operations in inland refineries

Chen, X. *et al. Computers & Chemical Engineering*, 2012, 44, 141–167.

This work presents a comparative analysis of the state-of-the-art multiple time-grid representations and formulations for the crude oil scheduling problem in inland refineries. The authors compare the event-based model, the unit slot model and the multi-operations sequence (MOS) model. Pros and cons of different models are highlighted based on modelling and computational experiments. The authors also propose several extensions of the previous models. The MOS model solved the problem much faster comparing to the other two models, but failed to find the best solution of some problems.

13/00696 Application of Bayesian in determining productive zones by well log data in oil wells

Masoudi, P. *et al. Journal of Petroleum Science and Engineering*, 2012, 94–95, 47–54.

Exploration specialists conventionally utilize a cut-off-based method to find productive zones inside the oil wells. Using conventional method, pay zones are separated crisply from non-pay zones by applying cut-off values on some petrophysical features. In this paper, a Bayesian technique is developed to find productive zones (net pays), and Bayesian network is used to select the most appropriate input features for this newly developed method. So, two Bayesian methods were developed: the first one with conventional pay determination inputs (shale percentage, porosity and water saturation), the other with two inputs, selected by Bayesian network (porosity and water saturation). Two developed Bayesian methods are applied on well log dataset of two wells: one well is dedicated for training and testing Bayesian methods, the other for checking generalization ability of the proposed methods. Outputs of two presented methods were compared with the results of conventional cut-off-based method and production test results (i.e. a direct procedure to check validation of proposed methods). Results show that the most prominent advantage of developed Bayesian method is determination of net pays fuzzily with no need to identify cut-offs, in addition to higher precision of classification: nearly 30% improvement in precision of determining net pays of first well (training well), and about 50% improvement in precision of determining productive zones through the generalizing well.

13/00697 Characterization and treatment of dissolved organic matter from oilfield produced waters

Wang, X. *et al. Journal of Hazardous Materials*, 2012, 217–218, 164–170.

Dissolved organic matter (DOM) has been studied intensively in streams, lakes and oceans due to its role in the global carbon cycle and because it is a precursor of carcinogenic disinfection by-products in drinking water; however, relatively little research has been conducted on DOM in oilfield produced waters. In this study, recovery of DOM from two oilfield produced waters was relatively low (~34%), possibly due to the presence of high concentrations of volatile organic compounds (VOCs). A van Krevelen diagram of the extracted DOM suggested the presence of high concentrations of lipids, lignin, and proteins, but low concentrations of condensed hydrocarbons. Most of the compounds in the oilfield DOM contained sulfur in their structures. Fourier transform infrared (FTIR) spectra indicated the presence of methyl groups, amides, carboxylic acids, and aromatic compounds, which is in agreement with results of Fourier transform ion cyclotron resonance (FT-ICR) analysis. Qualitatively, DOM in oilfield produced waters is similar to that reported in oceans and freshwater, except that it contains much more sulfur and is less aromatic. Treatment studies conducted in a fluidized bed reactor suggested that volatilization of organics may be a more important mechanism of DOM removal than microbial degradation.

13/00698 Dynamic risk assessment of oil spill scenario for Three Gorges Reservoir in China based on numerical simulation

Bi, H. and Si, H. *Safety Science*, 2012, 50, (4), 1112–1118.

A novel method for dynamic risk assessment of oil spill accidents based on numerical simulation was presented in this paper. The dynamic risk assessment model was developed consisting of a comprehensive list of caused consequences like environmental damage, asset loss, health impact and social effect as well as emergency actions preventing these losses. Contributing events in the master logic diagram of the dynamic risk assessment model were valued based on the simulated evolvement of oil contaminants under spill scenario on quasi-static fluid, which was obtained by coupling an oil spill model with hydrodynamic module in Jialing river of Three Gorges Reservoir in China after the impoundment of the reservoir to 175 m water level in 2010. The calculated result of dynamic risk as grade IV, which indicated that the assessed oil spill was not as catastrophic as thought because of the slow transport of oil fractions on water surface and absence of dispersed oil in water body due to the quasi-static fluid, very gentle wind and effective emergency actions, as well as by the reason that rare agriculture or industrial crops exist in spill adjacent area.

13/00699 Edgeworth price cycles and intertemporal price discrimination

Noel, M. D. *Energy Economics*, 2012, 34, (4), 942–954.

In a retail gasoline market exhibiting Edgeworth price cycles, prices change asymmetrically with many small decreases interrupted by occasional large increases. The result is a *de facto* menu of prices from which consumers can choose based on exactly when they buy. This article introduces four classes of purchase timing strategies designed to systematically shift consumer purchases towards the cycle troughs. It shows in the study market of Toronto, Canada, the monetary gains to consumers from optimized timing strategies are as high as 3.9%. Markups earned from these consumers fall up to 82%. In spite of the gains from timing strategies, surprisingly few consumers use them. Evidence is presented that a main reason is that consumers are not well informed about the cycles. Policy implications are discussed.

13/00700 Quantitative risk analysis of oil and gas drilling, using Deepwater Horizon as case study

Skogdalen, J. E. and Vinnem, J. E. *Reliability Engineering & System Safety*, 2012, 100, 58–66.

According to the National Commission on the BP Deepwater Horizon Oil Spill and Offshore Drilling, the Macondo blowout requires a reassessment of the risks associated with offshore drilling. The Commission recommends a proactive, risk-based performance approach specific to individual facilities, operations and environments, similar to the safety case/quantitative risk analysis (QRA) approach in the North Sea. A review of 15 QRAs from the North Sea reveals that the analyses to a large extent only to calculate the frequency of blowout based on the number of drilling operations. None of the reviewed analyses were initiated based on risk influence factors (RIFs) uncovered in the conceptual phase of well planning. The QRAs do not include human and organizational factors (HOFs). As seen in the Macondo blowout, most of the findings were related to HOFs, e.g. working practice, competence, communication, procedures and management. The narrow drilling window related to deepwater drilling has to be controlled by safety barriers that are dependent on HOFs. There is some research relating to the incorporation of HOFs in QRAs. Further improvements in methodology and datasets are necessary to ensure that the QRAs are valid for the individual facilities, operations and environments.

13/00701 Relationship between shoreline substrate type and sensitivity of seafloor habitats at risk to oil pollution

Leiger, R. *et al. Ocean & Coastal Management*, 2012, 66, 12–18.

The aim of this paper is to study the relationship between the shoreline substrate type, the shoreline substrate sensitivity (*in sensu* the environmental sensitivity index) and associated seafloor habitat's sensitivity (sensitivity of macrophytes and associated benthic invertebrates) to potential oil pollution in Tallinn Bay, the Baltic Sea. The sensitivity values of the seafloor habitats significantly differed among the studied shoreline substrate types, while the habitat sensitivity values did not match with the sensitivities of these substrate types. The average habitat sensitivity was high on shallow coastal sea adjoining cliffs (representing the shoreline substrate of lowest sensitivity), intermediate on till shores (the shoreline substrate of high sensitivity), low on sandy shores (the shoreline substrate of medium–low sensitivity) and artificial shores (the shoreline substrate of low sensitivity). This mismatch is explained by the fact that shoreline substrate sensitivity is a consequence of the shoreline natural persistence of oil and ease of cleanup, while the underwater habitat heterogeneity and community properties determine the sensitivity of the associated seafloor habitats to potential oil pollution. The layers of shoreline substrate types and seafloor habitat sensitivity are seen as elements of the environmental sensitivity index being developed for the Baltic Sea.

13/00702 Total factor productivity growth and convergence in the petroleum industry: empirical analysis testing for convexity

Kerstens, K. and Managi, S. *International Journal of Production Economics*, 2012, 139, (1), 196–206.

While economic theory acknowledges that some features of technology (e.g. indivisibilities, economies of scale and specialization) can fundamentally violate the traditional convexity assumption, almost all empirical studies accept the convexity property on faith. In this contribution, the authors apply two alternative flexible production technologies to measure total factor productivity growth and test the significance of the convexity axiom using a non-parametric test of closeness between unknown distributions. Based on unique field level data on the petroleum industry, the empirical results reveal significant differences, indicating that this production technology is most likely non-convex. Furthermore, the authors also show the impact of convexity on answers to traditional convergence questions in the productivity growth literature.

Derived liquid fuels

13/00703 Correlations for pour point and cloud point of middle and heavy distillates using density and distillation temperatures

Maheshwari, A. S. and Chellani, J. G. *Fuel*, 2012, 98, 55–60.

Pour point and cloud point are important parameters for a fuel especially the middle and heavy distillates. Therefore, good correlations for the same are of significant importance. Linear- and ANN-based correlations have been proposed for pour point and cloud point of mixtures. Linear correlations are simple and easy to use however errors for these correlations are higher than ANN based. For pour point the best correlation was ANN with seven weights and for cloud point, ANN with 25 weights. The linear correlation shows the dependency of pour point and cloud point with each of the chosen property from which it can also be concluded that the close relationship between these two. Also a robust correlation for both pour point and cloud point was found in the form of ANN with an average absolute error of 3.77 and 3.58 °C, respectively. These correlations can be easily employed for property estimation based on user's requirements of performance or accuracy.

13/00704 FTS fuels production over different Co/SiC catalysts

de la Osa, A. R. *et al. Catalysis Today*, 2012, 187, (1), 173–182.

The technical feasibility for Fischer–Tropsch synthetic fuels production over different cobalt/SiC catalysts was studied. Silicon carbide-supported catalysts were prepared by means of incipient wetness impregnation (IWI) and characterized by N_2 adsorption/desorption, acid/base titrations, XRD, TEM, TPR and pulse oxidation techniques. The bench scale catalytic performance was examined at a total pressure of 20 bar, a temperature range between 220 and 250 °C, a space velocity (GHSV) of $6000\,\mathrm{N\,cm^3\,g^{-1}\,h^{-1}}$ and using syngas with H_2/CO molar ratio equal to 2. For SiC-supported catalysts, the use of a certain amount of calcium as promoter resulted in a higher basicity and a slight higher cobalt dispersion. Furthermore, particle size and the degree of reduction were found to be directly influenced by the cobalt loading. A maximum extent of reduction was found at 12–15 wt% cobalt with little dependence on the addition of promoter. Catalytic activity provided promising Fischer–Tropsch performance with C_5^+ selectivity values higher than 90% in all the cases and especially on promoted catalysts (higher than 95%). In addition, promoted catalysts shifted C_5^+ hydrocarbon product distribution to higher molecular weight demonstrating that different commercial synthetic fuels formulations (gasoline to diesel) can be provided by modifying *m*Co-*n*Ca/SiC catalyst composition.

13/00705 Global optimization of a MINLP process synthesis model for thermochemical based conversion of hybrid coal, biomass, and natural gas to liquid fuels

Baliban, R. C. *et al. Computers & Chemical Engineering*, 2012, 42, 64–86.

A global optimization framework is proposed for a thermochemical based process superstructure to produce a novel hybrid energy refinery which will convert carbon-based feedstocks (i.e. coal, biomass and natural gas) to liquid transportation fuels. The mathematical model for process synthesis includes simultaneous heat, power, and water integration and is formulated as a mixed-integer non-linear optimization (MINLP) problem with non-convex functions. The MINLP model is large scale and includes 15,439 continuous variables, 30 binary variables, 15,406 equality constraints, 230 inequality constraints, and 335 non-convex terms. The non-convex terms arise from 274 bilinear terms, one quadrilinear term, and 60 concave cost functions. The proposed framework utilizes piecewise linear under-estimators for the non-convex terms to provide tight relaxations when calculating the lower bound. The bilinear terms are relaxed using a partitioning scheme that depends logarithmically on the number of binary variables, while the concave functions are relaxed using a linear partitioning scheme. The framework was tested on 12 case studies featuring three different plant capacities and four different feedstock-carbon conversion percentages and is able to solve each study to within a 3.22–8.56% optimality gap after 100 CPU hours. For 50% feedstock carbon conversion, the proposed global optimization framework shows that the breakeven oil prices for liquid fuels production are $61.36/bbl for the small case study, $60.45/bbl for the medium case study, and $55.43/bbl for the large case study, while the corresponding efficiencies are 73.9%, 70.5% and 70.1%, respectively.

13/00706 Improvement of the heats of reaction in endothermic reactions of methylcyclohexane with zeolites

Kim, J. *et al. Catalysis Today*, 2012, 185, (1), 47–53.

Endothermic reactions of methylcyclohexane (MCH) with zeolites were investigated in a batch reactor to increase the heats of reaction. Conversion and product distribution affected the heat of reaction. The heat of reaction with HZSM-5, which led to the formation of low-molecular-weight hydrocarbon products, was larger than the heats of reaction with other zeolites. To improve the heat of reaction with HZSM-5, Pt/HZSM-5 (1 wt% Pt) was used in endothermic reactions. In endothermic reactions with Pt/HZSM-5, the heats of reaction increased, and there was a high yield of olefins, which were formed by dehydrogenation of paraffin on metal sites. A high conversion and high yield of low-molecular-weight hydrocarbons and olefins led to an increase in the heat of reaction.

13/00707 Optimization strategy for long-term catalyst deactivation in a fixed-bed reactor for methanol synthesis process

Fuad, M. N. M. *et al. Computers & Chemical Engineering*, 2012, 44, 104–126.

In this study, the application of a repeated process estimation–optimization strategy is investigated for a methanol synthesis reactor system in the presence of a slowly deactivating catalyst. The purpose of this strategy is to update the optimal transition of the control variable profile with feedback from the process measurements. A state and parameter estimation method is formulated where the objective is to determine the current reactor state and model parameter from available process measurements data. In this strategy, the corresponding optimization problems are formulated as DAE-constrained optimization problems that are solved by using full discretization and large-scale NLP solver. Simulation results indicate that the strategy is able to track the theoretical optimum profile of the selected control variable as the catalyst deactivates. Moreover, with the formulated strategy, the performance of the reactor system in the presence of a long-term catalyst deactivation and unexpected plant operational changes can be improved significantly.

13/00708 Oxygen free conversion of natural gas to useful hydrocarbons and hydrogen over monometallic Mo and bimetallic Mo–Fe, Mo–Co or Mo–Ni/HZSM-5 catalysts prepared by mechanical mixing

Aboul-Gheit, A. K. *et al. Fuel Processing Technology*, 2012, 102, 24–29.

This work aims to approach a compromise of the activities of Mo/HZSM-5 catalyst as a well-known high performance aromatization catalyst after substituting half its Mo with Fe, Co or Ni (well-known active hydrogen releasing metals) for hydrocarbons and hydrogen production. The catalysts were prepared by the mechanical mixing procedure in order to keep the zeolitic pores almost free of metal incorporation and hence reducing the metal/zeolite acid interaction. The catalytic performance of the catalysts was investigated during the non-oxidative conversion of natural gas to hydrocarbons and hydrogen in a fixed bed flow reactor at 700 °C and gas hourly space velocity (GHSV) of 1500 ml/g/h. The catalysts were characterized by XRD and TGA, where the results showed that the bimetallic 3%Mo-3%Fe, 3%Mo-3%Co or 3%Mo-3%Ni containing catalysts significantly decreased hydrocarbon (ethylene and aromatics) yield and selectivity as compared to the monometallic 6%Mo/HZSM-5 catalyst. The substitution of group VIII metals enhances the rate of coke and hydrogen formation in the direction of going from Fe → Co → Ni. This behaviour can be attributed to the electronic properties of these metals, where maximum reaction rates are exhibited by the metals with six to eight d-electrons.

13/00709 Photocatalytic conversion of carbon dioxide into methanol using optimized layered double hydroxide catalysts

Ahmed, N. *et al. Catalysis Today*, 2012, 185, (1), 263–269.

The photocatalytic reduction of carbon dioxide into methanol was enabled between the Zn–Ga or Zn–Cu–Ga hydroxide layers using hydrogen and was promoted by the partial desorption of structural water stuffed between the cationic layers. The photoreduction rate obtained using $[Zn_{1.5}Cu_{1.5}Ga(OH)_8]_2^+\ (CO_3)^{2-} \cdot mH_2O$ was improved by replacing interlayer carbonate anions with $[Cu(OH)_4]^{2-}$ to $0.49\,\mu mol_{Methanol}\,h^{-1}\,g_{cat}^{-1}$, and the methanol selectivity was 88 mol%. At the molar level, interlayer Cu species was 5.9 times more active than the octahedral Cu sites in the cationic layers. The bandgap value was evaluated as 3.0 eV for the semiconductor $[Zn_{1.5}Cu_{1.5}Ga(OH)_8]_2^+\ [Cu(OH)_4]^{2-} \cdot mH_2O$. Direct electronic transition from O 2p to metal 3d, 4s, or 4p was responsible for the photocatalysis excited largely by ultraviolet light and to a lesser extent by visible light.

13/00710 Production of aromatics from heavier *n*-paraffins on hybrid cracking-reforming catalyst

Kimura, T. *et al. Catalysis Today*, 2012, 185, (1), 119–125.

Selective production of aromatics from the heavier *n*-paraffins was studied on nano-structured (*ns*) catalysts consisting of *ns* alumina and MFI-type H-galloaluminosilicate (H-GaAlMFI) zeolite. Performance of the hybrid H-GaAlMFI zeolite catalyst with *ns* Al_2O_3 was improved considerably from those of the zeolite sole catalyst and USY or H-ZSM-5 catalyst. It was observed that in the n-$C_{16}H_{34}$ conversion, the product selectivity for aromatics (including intermediate olefins and byproducts) and the degradation rate depended on either the ratios of Ga/(Ga + Al) and Si/(Ga + Al) in the zeolite component or on the co-existence of *ns* Al_2O_3. It was found that aromatics could be produced selectively by controlling the reaction time. In regards to the catalytic active sites, the *ns* species at the zeolite surface layer and the surface distributions were confirmed by X-ray photoelectron spectroscopy with the Ar-etching method. It was determined that non-framework Ga species existed as Ga oxides after calcining. It was also revealed that the *ns* alumina had an important role in forming the *ns* species of non-framework Ga by extracting it from the zeolite framework and stabilizing it as an *ns* oxide at the zeolite particle surface which opened into the nano-space.

13/00711 Sewage sludge pyrolysis for liquid production: a review

Fonts, I. *et al. Renewable and Sustainable Energy Reviews*, 2012, 16, (5), 2781–2805.

The high output of sewage sludge, which is increasing during recent years, and the limitations of the existing means of disposing sewage sludge highlight the need to find alternative routes to manage this waste. Biomass and residues like sewage sludge are the only renewable energy sources that can provide C and H, thus it is interesting to process them by means of treatments that enable to obtain chemically valuable products like fuels and not only heat and power; pyrolysis can be one of these treatments. The main objective of this review is to provide an account of the state of the art of sewage sludge pyrolysis for liquid production, which is under study during recent years. This process yields around 50 wt% (daf) of liquid. Typically, this liquid is heterogeneous and it usually separates into two or three phases. Some of these organic phases have very high gross heating values, even similar to those of petroleum-based fuels. The only industrial sewage sludge pyrolysis plant operated to date is currently closed due to some technical challenges and problems of economic viability.

13/00712 Study of the interfacial forces and turbulence models in a bubble column

Silva, M. K. *et al. Computers & Chemical Engineering*, 2012, 44, 34–44.

Three-dimensional Eulerian simulations of gas–liquid flows in a cylindrical bubble column were performed in order to evaluate the flow pattern in the heterogeneous flow regime. Simulations were conducted numerically by the finite element method using a commercial CFX code (v.12.0) and an analysis of interfacial forces such as drag, lift and turbulent dispersion, as well as a comparison of k–ε and Reynolds stress (RSM) turbulence models were performed. Different bubble sizes and two boundary conditions for the column exit were also verified. Gas velocities and holdup profiles were compared with experimental data. Results have shown that at the sparger region and without any simplification on the boundary condition the RSM model better represents the flow. At the fully developed region k–ε also showed good results.

03 GASEOUS FUELS

Sources, properties, recovery, treatment

13/00713 Acoustic evidence for a gas migration and release system in Arctic glaciated continental margins offshore NW-Svalbard

Rajan, A. *et al. Marine and Petroleum Geology*, 2012, 32, (1), 36–49.

High-resolution 3D and 2D seismic data offshore northwest Svalbard, west of Prins Karls Forland, provide geophysical evidence for geologically controlled fluid migration pathways, gas hydrate occurrence, and an active seabed gas expulsion system. The investigated seabed area covers ~1600 km^2 and lies between Kongsfjorden cross-shelf trough in the north and Isfjorden cross-shelf trough in the south ranging in water depths from ~200 m on the shelf to 800 m on the upper continental slope. Acoustic evidence for present day methane release from the seabed to the water column comes from more than 220 gas flares at the outer shelf while past methane release activity at the mid-shelf area is evident from pockmarks without flares. The fluid migration pathways towards the seabed can be drawn from sub-seabed acoustic anomalies. Fluid migration towards the upper slope occurs mostly along strata in upslope direction and largely prevails over vertical focused migration. Fluids accumulate in the uppermost part of the slope just westward of the shelf break, where they are trapped beneath the prograding glacigenic sequence, which is not permeable enough for fluids to migrate through. Fluids are expelled on the shelf where the base of the glacigenic sequence outcrops. Some gas-charged fluids may originate from deep-seated hydrocarbon reservoirs and can be temporally stored in gas hydrates in the shallow subsurface. Though evidence for hydrates on the uppermost slope is missing the seismic data from the lower slope clearly suggest the occurrence of gas hydrate.

13/00714 Adhesion, plasticity and other peculiar properties of solid methane

Kirichek, O. *et al. Cryogenics*, 2012, 52, (7–9), 325–330.

Adhesion and plasticity of polycrystalline solid methane have been studied in the temperature range 10–90 K. It was shown that adhesion is very strong in the 50–90 K temperature range where the solid methane is soft and sticky. Closer to the melting point (at 90.6 K) the solid methane behaves as extremely viscous non-Newtonian liquid. Below 30 K solid methane loses its stickiness and ductility and acts like ordinary glass. Methane adhesion remains similar for very different materials. The authors have also made some video observations which reveal unexpected and mostly inexplicable properties of solid methane which could be of some interest for designing new methane moderators for neutron sources and planetary physics particularly the study of the environment of Titan.

13/00715 Correlation and prediction of the solubilities of solid *n*-alkanes in supercritical carbon dioxide using the Carnahan–Starling–van der Waals model with a density-dependent parameter

Li, H. *et al. Fluid Phase Equilibria*, 2012, 325, 28–34.

In this paper, the solubilities of some solid *n*-alkanes in supercritical carbon dioxide were correlated and predicted using the Carnahan–Starling–van der Waals model with a density-dependent parameter of a_{12}. It was found that the parameter values of a_{12} for solid *n*-alkanes in CO_2 at different temperatures are equal at the crossover pressure of 24 MPa, and a_{12} can be correlated with carbon number of the corresponding solid *n*-alkanes. At a given temperature, the linear fit of parameters a_{12} versus the density of the solvent was used for solubility correlation, resulting in an average absolute average relative deviation of 11.82%, which is comparable with that of the Peng–Robinson equation of state combined with the van der Waals two-parameter mixing rule model. The regressed slope *m* and intercept *n* of the linear fit can also be correlated with the carbon number of solid *n*-alkanes. The solubilities of solid *n*-alkanes can be predicted with a_{12} at the crossover pressure and slope *m* or with intercept *n* and slope *m*.

13/00716 Development of a multi-mechanistic, dual-porosity, dual-permeability, numerical flow model for coalbed methane reservoirs

Thararoop, P. *et al. Journal of Natural Gas Science and Engineering*, 2012, 8, 121–131.

Most existing coalbed methane (CBM) simulators usually treat coal seams as dual-porosity, single-permeability systems ignoring the effects of water presence in the coal matrix. In this study, a compositional dual-porosity, dual-permeability CBM simulator has been developed. The CBM reservoir is treated as a dual-porosity, dual-permeability system consisting of coal matrix and fracture network. The development of the proposed numerical model incorporates the effects of water presence in the coal matrix and the phenomena of coal shrinkage and swelling. The transport of gas follows a multi-mechanistic flow mechanism triggered by pressure and concentration gradients. In addition, the proposed simulator is able to collapse to simpler coal seam representations and was successfully tested against the existing commercial and research CBM simulators for CO_2-enhanced CBM recovery process. Successful history matching exercises were performed on pure CO_2 injection and flue gas injection using the actual field data.

13/00717 Evaluation of marine biomass as a source of methane in batch tests: a lab-scale study

Gurung, A. *et al. Energy*, 2012, 43, (1), 396–401.

Marine biomass is considered an important feedstock for anaerobic digestion to generate energy; however, its utilization as an energy source is still minimal around the world. In the current study, the biochemical methane potential test was used to evaluate energy recovery from seaweed, brown algae, green algae, and fish viscera as substrates for methane production. Cumulative CH_4 yields of 256 ± 28 and 179 ± 35 mL CH_4/g VS were observed using green and brown algae, respectively, after 60 days of digestion. The CH_4 content of the biogas was approximately 70% for both substrates. Lower CH_4 yields of 127 ± 20 and 102 ± 25 mL CH_4/g VS were observed using fish viscera and seaweed, respectively. Given that $44 \pm 15\%$ of the TCOD was converted to CH_4, a longer adaption period or pretreatment of the marine biomass is necessary to fully convert the TCOD to CH_4.

13/00718 Fracture development in shale and its relationship to gas accumulation

Ding, W. *et al. Geoscience Frontiers*, 2012, 3, (1), 97–105.

Shale with high quartz, feldspar and carbonate, will have low Poisson's ratio, high Young's modulus and high brittleness. As a result, the shale is conducive to produce natural and induced fractures under external forces. In general, there is a good correlation between fracture development in shale and the volume of brittle minerals present. Shale with high TOC or abnormally high pressure has well-developed fractures. Shale fracture development also shows a positive correlation with total gas accumulation and free gas volume, i.e. the better shale fractures are developed, the greater the gas accumulation and therefore the higher the gas production. Fractures provide migration conduits and accumulation spaces for natural gas and formation water, which are favourable for the volumetric increase of free natural gas. Wider fractures in shale result in gas loss. In North America, there is a high success ratio of shale gas exploration and high gas production from high-angle fracture zones in shale. Good natural gas shows or low yield producers in the Lower Paleozoic marine organic matter-rich rocks in the Sichuan Basin are closely related to the degree of fracture development in brittle shales.

13/00719 Geochemical evolution of organic-rich shales with increasing maturity: a STXM and TEM study of the Posidonia Shale (Lower Toarcian, northern Germany)

Bernard, S. *et al. Marine and Petroleum Geology*, 2012, 31, (1), 70–89.

Hydrocarbon generation and retention processes occurring within gas shales as a response to increases in thermal maturation are still poorly constrained. While efforts have been directed at unravelling the resource potential, composition and textures of these economically important unconventional systems, their spatial variability in chemistry and structure is still poorly documented at the sub-micrometre scale. Here, the authors have characterized samples of the Lower Toarcian Posidonia Shale samples from northern Germany at varying stages of thermal maturation using a combination of compositional organic geochemistry and spectromicroscopy techniques, including synchrotron-based scanning transmission X-ray microscopy. They document geochemical and mineralogical heterogeneities down to the nanometre scale within the investigated samples as a function of their level of thermal maturity. In particular, authigenic albite crystals containing nanometric halite inclusions have been documented within the investigated mature and overmature samples. The presence of such tracers of palaeobrine–carbonate interactions supports a maturation scenario for the Lower Toarcian Posidonia Shale intimately related to ascending brine fluids rather than a maturation scenario solely resulting from high heat flows. In addition, various types of asphaltene- and NSO-rich bitumen have been detected within the same samples, very likely genetically derived from thermally degraded organic precursors. Furthermore, the formation of nanoporous pyrobitumen has been inferred for samples of gas window maturity, likely resulting from the formation of gaseous hydrocarbons. By providing *in situ* insights into the fate of bitumen and pyrobitumen as a response to the thermal evolution of the macromolecular structure of kerogen, the results reported here constitute an important step towards better constraining hydrocarbon generation processes during natural shale gas maturation.

13/00720 Influence of super-absorbent polymer on the growth rate of gas hydrate

Wu, Q. *et al. Safety Science*, 2012, 50, (4), 865–868.

The growth rate of hydrate and morphology of methane hydrate formation were studied in a visual pressure cell at 5.5 MPa. The gas hydrate formation was carried out (coal mine methane (CMM) + tetrahydrofuran (THF) + sodium dodecyl sulfate (SDS) + H_2O) with and without SAP. Experimental data on the hydrate growth rate and induction time were obtained for three different CMM samples. The influence of SAP on hydrate growth rate was determined. Results showed that after the addition of SAP, with the methane concentration increased in CMM, the induction time was reduced by 9, 10 and 3 min, and the growth rate was shortened by 0.56×10^{-6}, 0.53×10^{-6} and 1.42×10^{-6}/m^3 min^{-1}, respectively. This study could be useful for the recovery of methane from CMM by forming hydrate in the chemical and mining industry.

13/00721 Introducing new method to improve log derived saturation estimation in tight shaly sandstones – a case study from Mesaverde tight gas reservoir

Amiri, M. *et al. Journal of Petroleum Science and Engineering*, 2012, 92–93, 132–142.

Relative permeability studies performed on tight gas sand core show that water saturation has much influence upon effective gas permeability. This makes water saturation in tight gas sand a critical reservoir parameter. The aim of this study is to introduce a new approach to reduce uncertainty in water saturation estimation using well logs models in tight gas shaly sandstones. This paper consists of two parts. The first part gives introduction on the Indonesian model as the most reliable model for prediction of water saturation in this reservoir type because it has the least uncertainty if the least-square error method (LSE) among six frequently used conventional water saturation models is deployed (i.e. total shale, modified total shale, Indonesian, dispersed clay, simandoux and modified simandoux). The authors develop a new method in the second section to present an equation that could improve the Indonesian model. This equation is presented through resistivity, gamma ray, neutron and density logs, which are the common available logs in most of the wells and formations under study. In this study, 14 wells (in 39 different zones) from five basins of Mesaverde tight gas sandstones across western US basins were chosen in order to demonstrate the reliability of this method. The equation that is introduced in this study has shown good performance in improving the estimation of water saturation in 85% of the total zones (i.e. 33 zones out of 39).

13/00722 On some studies about the dynamic mechanisms of carbon monoxide flow and diffusion during high energy gas fracturing

Pu, J. *et al. Safety Science*, 2012, 50, (4), 903–908.
The high-energy gas fracturing (HEGF) technique has been one of the central stimulating measures to enhance oil recovery in low permeability reservoirs. But, in recently few years, some serious CO poisoning accidents have taken place in oilfields in China. It is very important to reveal the dynamic mechanisms of carbon monoxide flow and diffusion to operating safety during high energy gas fracturing. In this paper, some dynamic mechanisms of carbon monoxide flowing inside an oil wellbore and diffusion on the top of the well during high energy gas fracturing were studied with fluid/gas hydrodynamics. The CO flow model within a wellbore and the diffusion model in air were established. The key factors affecting CO flow and diffusion such as wellbore pressure, gas–oil ratio, wind speed, leakage speed, air-permanence were inspected with mathematical simulation. This research will be of significance to provide an important guidance for monitoring and preventing CO poisoning accidents during HEGF.

13/00723 Sensitivity analysis of gas production from class I hydrate reservoir by depressurization

Jiang, X. *et al. Energy*, 2012, 39, (1), 281–285.
A 3D numerical model for gas production from hydrate reservoirs is developed, which considers kinetics of dissociation, heat and multi-phase fluid flow. Three components (gas, water and hydrate) and three phases (gas, water and hydrate) are considered in the model. The equations are spatially discretized by a finite difference method. IMPES method is used to solve the mass balance equations and temperature is solved implicitly. Based on the model, gas production from class I hydrate reservoir (with underlying free gas) under constant bottom-hole pressure was simulated. The sensitivity analysis of the factors including development parameters and reservoir parameters were performed. Results show that hydrate dissociation rate increases with the increases of initial reservoir temperature. The larger the absolute permeability is, the higher the hydrate dissociation rate is. Hydrate dissociation rate is significantly improved, when dissociation rate constant increases. However, higher initial reservoir pressure and bottom-hole pressure will lead to lower hydrate dissociation rate. Research results provide theoretical support for hydrate production.

13/00724 State of the art: natural gas hydrates as a natural resource

Koh, C. A. *et al. Journal of Natural Gas Science and Engineering*, 2012, 8, 132–138.
An overview is provided of the 800 papers presented at the Seventh International Conference on Gas Hydrates, 2011, to demonstrate the basic chemico-geophysics, as well as a perspective on hydrates as a resource activity by each country. The following summarizes the current status of gas hydrates as a natural resource: (1) there is substantial methane in hydrates, (2) the most accessible hydrates are in sandy sediments, with lithological controls, (3) laboratory characterization tools are available, (4) field detection tools are acceptable, (5) many of the national programs are in the phase of resource identification and characterization, with two exceptions, and (6) the first long-term production tests of methane hydrates will likely start in 2012 in the north slope permafrost, and offshore Japan.

13/00725 Stochastic modelling of coalbed methane resources: a case study in Southeast Qinshui Basin, China

Zhou, F. *et al. International Journal of Coal Geology*, 2012, 99, 16–26.
This paper presents a stochastic analysis of coalbed methane (CBM) resources for a coal seam in south-east Qinshui Basin, China. Log and laboratory data are used to predict the coal thickness, coal ash content and coal gas content. Using reservoir modelling, the distributions of the karst collapse column (KCC), coal seam thickness, coal quality and coal gas content are generated. The convergent interpolation and sequential Gaussian simulation methods are used to model the surface and structure of the coal seam. The structural models are determined by the surface structure and coal seam thickness. Based on the structural models, the coal and KCC are converted to two facies and their distributions are obtained using object modelling. The coal density distributions are simulated based on each facies model using the sequential Gaussian simulation. Finally, different realizations are used to study CBM resources. The results show that the heterogeneities in coal seam thickness and coal quality lead to significant uncertainty in estimating CBM resources. A model with lower heterogeneity gives a greater CBM resource. The distributions of KCC, coal seam thickness, coal quality and gas content are the main sources for uncertainty in CBM resource estimation. The density variogram and top structure contribute less to the uncertainty in CBM resources.

13/00726 Subsurface gas hydrates in the northern Gulf of Mexico

Boswell, R. *et al. Marine and Petroleum Geology*, 2012, 34, (1), 4–30.
The northern Gulf of Mexico (GoM) has long been a focus area for the study of gas hydrates. Throughout the 1980s and 1990s, work focused on massive gas hydrates deposits that were found to form at and near the seafloor in association with hydrocarbon seeps. However, as global scientific and industrial interest in assessment of the drilling hazards and resource implications of gas hydrate accelerated, focus shifted to understanding the nature and abundance of ‘buried’ gas hydrates. Through 2005, despite the drilling of more than 1200 oil and gas industry wells through the gas hydrate stability zone, published evidence of significant sub-seafloor gas hydrate in the GoM was lacking. A 2005 drilling program by the GoM Gas Hydrate Joint Industry Project (the JIP) provided an initial confirmation of the occurrence of gas hydrates below the GoM seafloor. In 2006, release of data from a 2003 industry well in Alaminos Canyon 818 provided initial documentation of gas hydrate occurrence at high concentrations in sand reservoirs in the GoM. From 2006 to 2008, the JIP facilitated the integration of geophysical and geological data to identify sites prospective for gas hydrate-bearing sands, culminating in the recommendation of numerous drilling targets within four sites spanning a range of typical deepwater settings. Concurrent with, but independent of, the JIP prospecting effort, the Bureau of Ocean Energy Management (BOEM) conducted a preliminary assessment of the GoM gas hydrate petroleum system, resulting in an estimate of 607 trillion cubic metres (21,444 trillion cubic feet) gas-in-place of which roughly one-third occurs at expected high concentrations in sand reservoirs. In 2009, the JIP drilled seven wells at three sites, discovering gas hydrate at high saturation in sand reservoirs in four wells and suspected gas hydrate at low to moderate saturations in two other wells. These results provide an initial confirmation of the complex nature and occurrence of gas hydrate-bearing sands in the GoM, the efficacy of the integrated geological/geophysical prospecting approach used to identify the JIP drilling sites, and the relevance of the 2008 BOEM assessment.

13/00727 The influence of NaCl ions on hydrate structure and thermodynamic equilibrium conditions of gas hydrates

Qi, Y. *et al. Fluid Phase Equilibria*, 2012, 325, 6–10.
Concentrated brines are known to be very good inhibitors for gas hydrate formation, and gas hydrates can be used in the desalination of seawater under the assumption that salinity is zero in gas hydrates. However, its molecular mechanism has not been understood yet. The authors examined this by classical molecular dynamics simulations. The simulations results showed that a pair of Na^+–Cl^- ions can be included in a unit cell of the hydrates with the hydrate structure being stable. However, the equilibrium pressure was larger than that of pure hydrates. Therefore, it is concluded that gas hydrates may not be salt-free completely, i.e., 0.07 wt% salinity at least. Furthermore, Na^+ ions have a smaller effect on the crystal structure deformation and the equilibrium pressure of the hydrates than Cl^- ions, as $4\,Na^+$ ions may be contained in a unit cell of the hydrates. Meanwhile, massive salt ions approach to concentrate on the surface of the hydrates. The simulation results are consistent with the available desalination experimental results utilizing gas hydrate method.

13/00728 Thermal behaviour modelling of a reference calorimeter for natural gas

Haloua, F. *et al. International Journal of Thermal Sciences*, 2012, 55, 40–47.
The French National Metrology and Testing Institute (LNE) build an isoperibolic reference gas calorimeter to measure the calorific value of natural gas with a high level of accuracy with the collaboration of the R&D division of GDF-Suez. With three-dimensional numerical modelling tools, GDF-Suez developed a comprehensive and refined model of the complete calorimeter geometry and evaluated the heat flux sources to reproduce the thermal behaviour of this calorimeter. The objectives are to optimize the thermal homogeneity and to maximize heat transfer to the water bath. The accurate assessment of the different thermal fluxes transferred to the water bath was performed based on a complete simulation of the combustion of the fuel gas in the burner. The numerical model results fit quite closely the experimental thermal behaviour of the calorimeter. The energy balance shows that approximately 90% of the total energy is absorbed by the water bath and about 10% by the calorimetric walls with a weak contribution of the radiative heat transfer to the calorimeter vessel. A comparative study between the numerical and experimental results confirms both that the geometries of the calorimeter vessels and the glass burner are adequate. The new refined geometric model validates

also the location of the thermal sensor in the bath. The expected outcome of both experiments and thermal modelling is to decrease the uncertainty of the calorific value measured with this standard combustion calorimeter.

13/00729 Tight gas sandstone reservoirs in China: characteristics and recognition criteria

Zou, C. *et al. Journal of Petroleum Science and Engineering*, 2012, 88–89, 82–91.

Tight gas sandstone (tight gas) reservoirs have been widely discovered in a number of basins in China including the Sichuan, Ordos, Turpan-Hami (Tuha), Songliao, Junggar, Tarim, Chuxiong and East China Sea basins. Genetically they are of either primary or secondary accumulations. The tight gas accumulations are mostly associated with coal strata. The reservoir rocks are mainly lithic arkosic sandstones and feldspathic lithic arenite. They are characterized by low compositional maturities, low cement contents and moderate petrological textural maturities. The diagenetic evolution of the reservoirs is generally at a high level, reaching the mid-late diagenesis stages. Reservoir porosities are dominated by secondary intragranular dissolution porosity and intergranular dissolution porosity with subordinate primary residual intergranular porosity. The pore throats are sheet like or bending-flake like in geometry and generally have poor connectivity. The tight gas reservoirs have poor petrophysical properties and show strong heterogeneities. Locally, some moderately porous and low permeable or low porous and moderately permeable sandstone reservoirs are present. Compaction and cementation appear to be key factors contributing to the formation of the tight gas sandstone reservoirs. Based on the synthesis of a vast data set obtained from some known tight sandstone gas accumulations from (1) the upper Palaeozoic sandstones in the Ordos Basin, (2) the Triassic Xujiahe Formation in the Sichuan Basin, (3) the Jurassic sandstones from the foothill belt in the Tuha Basin and (4) the Cretaceous deep reservoirs in the Songliao Basin, the criteria for recognizing tight gas sandstone reservoirs in China can be established as an *in situ* permeability of less than or equal to 0.1 mD and with no natural commercial production.

13/00730 Viscosity prediction for natural gas processing applications

Motahhari, H. *et al. Fluid Phase Equilibria*, 2012, 322–323, 56–65.

The expanded fluid (EF) viscosity correlation was used to model the viscosity of mixtures commonly encountered in natural gas processing. This correlation provides viscosity values as a function of fluid density and characterizes each pure compound with three fluid-specific parameters: c_2, $\rho^{O}{}_{S}$ and c_3, when using experimental densities (version 1) and two parameters, c_2 and $\rho^{O}{}_{S}$, when using a cubic equation of state (version 2). In particular, the original EF correlation for hydrocarbons was adapted for non-hydrocarbon components, including: carbon dioxide, hydrogen sulfide, nitrogen, helium, water, methanol, ethylene glycol, diethylene glycol and triethylene glycol. A temperature dependency was introduced for parameter c_2 for components with significant hydrogen bonding such as water and methanol. For all other components, a fixed c_2 was found to be adequate. Both versions of the correlation were fit to experimental data for the non-hydrocarbon components with overall average absolute relative deviation (AARD) below 6%. The viscosities of several sweet and sour natural gas mixtures were predicted with overall AARDs of 6.3% and 5.1% for versions 1 and 2, respectively. The viscosities of aqueous solutions both of methanol and of glycols were also modelled. A binary interaction parameter was required to fit the data for all aqueous mixtures in version 2 but only for mixtures of water and methanol in version 1. The overall AARDs of the calculated viscosities of the aqueous solutions of methanol and glycols by versions 1 and 2 were 6% and 8.7%, respectively.

Transport, storage

13/00731 A huff-and-puff production of gas hydrate deposits in Shenhu area of South China Sea through a vertical well

Su, Z. *et al. Journal of Petroleum Science and Engineering*, 2012, 86–87, 54–61.

The Shenhu area on the northern continental slope of the South China Sea is one of the most promising fields for gas hydrate exploitation. Drilling and sampling have indicated high saturations of methane hydrate in clay silty sediments at drilling site SH2. The hydrate-bearing layer is overlain and underlain by permeable zones of mobile water, and the system does not appear to be bounded by low-permeability strata. In this study a huff-and-puff method is used to produce gas from the hydrate accumulation. The authors simulated numerically hydrate dissociation and gas production by alternately injecting hot water and producing fluids at a vertical well. The simulations show the gas production rate in huff-and-puff operations is very small (50–140 m^3/d), and unacceptable for commercial production. The calculation also indicated secondary hydrates form at the very early period of injecting operations, and then gas is released due to the thermal stimulation of hot water, but the amount of released gas in the injection periods of hot water was much smaller than that converted into secondary hydrates. The study provides an insight into the production potential of the Shenhu hydrate accumulations through the huff-and-puff method, and a basis for the analysis of the economic feasibility of gas production from that area.

13/00732 Effect of residual stress on the integrity of a branch connection

Law, M. *et al. International Journal of Pressure Vessels and Piping*, 2012, 96–97, 24–29.

A new connection to an existing gas pipeline was made by hot-tapping, welding directly onto a pressurized pipeline. The welds were not post-weld heat treated, causing significant residual stresses. The critical weld had residual stresses determined by neutron diffraction using ANSTO's residual stress diffractometer, Kowari. The maximum measured residual stress (290 MPa) was 60% of the yield strength. The magnitudes of errors from a number of sources were estimated. An integrity assessment of the welded branch connection was performed with the measured residual stress values and with residual stress distributions from the BS 7910 and API 579 analysis codes. Analysis using estimates of residual stress from API 579 overestimated the critical crack size.

13/00733 Emergency venting into redundant pipelines

Ettouney, R. S. *et al. Journal of Loss Prevention in the Process Industries*, 2012, 25, (4), 739–745.

The evolution of pressure, temperature, and gas inventory during containment of blowdown from two high pressure gas networks into a third lower pressure relatively large redundant pipeline is followed through a simple lumped parameter model. Numerical solution of the non-linear model equations enabled to study the effects of relevant operating conditions on the system's dynamics. The effects of initial pressure difference between the supply and receiving networks, ratio of discharge orifice to pipe diameters in the supply networks, and heat transfer from the surroundings are investigated. A set of computer generated results are presented to demonstrate vividly the effect of the above variables on the percentage of gas recovered in the lower pressure pipeline, the blowdown time, and the minimum temperatures reached in the networks.

13/00734 Evaluation on gas production potential from laminar hydrate deposits in Shenhu area of South China Sea through depressurization using vertical wells

Su, Z. *et al. Journal of Petroleum Science and Engineering*, 2012, 86–87, 87–98.

Gas hydrates are solid crystalline compounds in which gas molecules are lodged in lattices of ice crystals. Shenhu area is considered as one of the most promising fields on north continental slope of the South China Sea (SCS). Drilling and sampling at the site has indicated occurrences of methane hydrate in clay silty sediments. The thin hydrate-bearing layer (HBL) is overlain and underlain by zones of mobile water, and the layer does not appear to be bounded by low-permeability strata. This study assesses by means of numerical simulation the production potential of the laminar hydrate deposit at drilling site SH3 in the Shenhu area. The authors simulate the hydrate dissociation and the gas production induced by depressurization at a vertical well. To minimize gas losses through the overburden and excessive water production through proximity to the permeable, water-saturated zones, a perforated interval is limited to the middle section of the vertical well within the hydrate layer. The simulations show that production from depressurization-induced dissociation through a vertical well at constant well pressure does not appear to be a promising approach in the deposits of low hydraulic diffusion. The production of hydrate-originating gas decreases at the beginning of the production and then stays stable in the reference case and the average production is 211 m^3/d. The deposit permeability is considered the most insensitive parameter to enhance the gas production. And the production potential is much lower than that of deposits having an impermeable upper boundary as expectation.

13/00735 Failure prediction for crack-in-corrosion defects in natural gas transmission pipelines

Bedairi, B. *et al. International Journal of Pressure Vessels and Piping*, 2012, 96–97, 90–99.

Cracks occurring coincidentally with corrosion (crack-in-corrosion or CIC), represent a new hybrid defect in pipelines that are not directly addressed in the current codes or assessment methods. To understand the failure response of these defects, the finite element method using an elastic–plastic fracture mechanics approach was applied to predict the failure pressures of comparable crack, corrosion and CIC defects in 508 mm diameter pipe with 5.7 mm wall thickness. Failure pressure predictions were made based on measured tensile, Charpy impact and J-testing data, and validated using experimental rupture tests. Plastic collapse was predicted for corrosion and crack defects using the critical strength based on the material tensile strength, whereas fracture was predicted using the measured $J_{0.2}$ value. The model predictions were found to be conservative for the CIC defects (17.4% on average), 12.4% conservative for crack-only defects, and 3.2% conservative for corrosion defects compared to the experimental tests, demonstrating the applicability of the material-based failure criteria. For the defects considered in this study, all were predicted to fail by plastic collapse. The finite element method provided less conservative predictions than existing corrosion or crack-based analytical methods.

13/00736 Inhibition of methane hydrate re-formation in offshore pipelines with a kinetic hydrate inhibitor

Seo, Y. and Kang, S. P. *Journal of Petroleum Science and Engineering*, 2012, 88–89, 61–66.

Methane gas from marine hydrate deposits can be produced by one or a combination of three methods; depressurization, thermal stimulation, and the injection of hydrate inhibitors. Because residual hydrate structures known as hydrate precursors will exist in the liquid water phase after dissociation, the risk of methane hydrate re-formation has to be evaluated during the production and transportation of methane gas through offshore pipelines. New experimental procedures composed of three stages are designed to simulate the dissociation of marine hydrates and the transportation of produced fluids. The obtained experimental results have shown that methane hydrates are rapidly re-formed when the temperature of dissociated water falls into the hydrate formation region during the cooling down process. The subcooling for three different dissociation pressures of 80, 70 and 60 bar were 1.3, 1.2 and 1.6 °C, respectively. One viable option to avoid hydrate re-formation is injecting hydrate inhibitors before transporting the fluids through pipelines. Among various hydrate inhibitors, poly(N-vinylcaprolactam) (PVCap) was selected as a possible candidate for a kinetic hydrate inhibitor (KHI) and injected into dissociated water before cooling down the fluids. The concentration of PVCap was varied from 0.5 to 3.0 wt%. With an increase in the PVCap concentration, the subcooling increased to 7.8 °C at a dissociation pressure of 80 bar, which suggests that the risk of hydrate re-formation can be reduced by injecting PVCap. Moreover it is observed that the subcooling increased to 8.8 °C at the PVCap concentration of 3.0 wt% in the presence of NaCl in the water phase. Although the use of KHI in conventional gas production has become common, its applicability to methane hydrate production has not yet been studied thoroughly, especially in the presence of residual hydrate structures. In this work, the application of a KHI to methane hydrate production is discussed.

13/00737 Numerical simulation and study on the transmission law of flame and pressure wave of pipeline gas explosion

Huang, Z. *et al. Safety Science*, 2012, 50, (4), 806–810.

Based on FLUENT simulation software, the laws of transmission of flame and pressure wave in pipeline gas explosion were studied. It turned out that, the maximum pressure value of the explosion point is not the maximum value of the whole explosion process; the maximum pressure value of the pressure wave lowers firstly near the explosion point, then rises to a peak, and then drops gradually; two waves divide the space in the pipeline into three sections during the gas explosion transmission. The result is basically consistent between numerical simulation and experiment, and the conclusion from the simulation provides theoretical basis for research on explosion-proof and suppression devices for underground gas pipeline, as well as for technical regulations of installation.

13/00738 Numerical simulations of depressurization-induced gas production from gas hydrate reservoirs at the Walker Ridge 313 site, northern Gulf of Mexico

Myshakin, E. M. *et al. Marine and Petroleum Geology*, 2012, 34, (1), 169–185.

In 2009, the Gulf of Mexico (GOM) Gas Hydrates Joint-Industry-Project (JIP) Leg II drilling program confirmed that gas hydrate occurs at high saturations within reservoir-quality sands in the GOM. A comprehensive logging-while-drilling dataset was collected from seven wells at three sites, including two wells at the Walker Ridge 313 site. By constraining the saturations and thicknesses of hydrate-bearing sands using logging-while-drilling data, two-dimensional (2D), cylindrical, *r-z* and three-dimensional (3D) reservoir models were simulated. The gas hydrate occurrences inferred from seismic analysis are used to delineate the areal extent of the 3D reservoir models. Numerical simulations of gas production from the Walker Ridge reservoirs were conducted using the depressurization method at a constant bottomhole pressure. Results of these simulations indicate that these hydrate deposits are readily produced, owing to high intrinsic reservoir-quality and their proximity to the base of hydrate stability. The elevated *in situ* reservoir temperatures contribute to high (5–40 MMscf/day) predicted production rates. The production rates obtained from the 2D and 3D models are in close agreement. To evaluate the effect of spatial dimensions, the 2D reservoir domains were simulated at two outer radii. The results showed increased potential for formation of secondary hydrate and appearance of lag time for production rates as reservoir size increases. Similar phenomena were observed in the 3D reservoir models. The results also suggest that interbedded gas hydrate accumulations might be preferable targets for gas production in comparison with massive deposits. Hydrate in such accumulations can be readily dissociated due to heat supply from surrounding hydrate-free zones. Special cases were considered to evaluate the effect of overburden and underburden permeability on production. The obtained data show that production can be significantly degraded in comparison with a case using impermeable boundaries. The main reason for the reduced productivity is water influx from the surrounding strata; a secondary cause is gas escape into the overburden. The results dictate that in order to reliably estimate production potential, permeability of the surroundings has to be included in a model.

13/00739 Production characteristics and the key factors in high-rank coalbed methane fields: a case study on the Fanzhuang Block, Southern Qinshui Basin, China

Lv, Y. *et al. International Journal of Coal Geology*, 2012, 96–97, 93–108.

The temporal and spatial production characteristics of coalbed methane (CBM) wells in the Fanzhuang Block of the Southern Qinshui Basin, the first commercial CBM-producing basin in China, were studied to determine the dominant factors. The study indicates that gas production differs significantly in different wells adjacent to or located in different tectonic areas. In combination with the production characteristics in the temporal and spatial variations, the impact of seven factors (burial depth, thickness of coal, gas content, porosity/permeability, effect of fracturing, structural setting, and hydrogeological conditions) on the gas production was analysed based on bivariate correlation analysis and grey system theory, which are suitable for solving the complex interrelationships between multiple factors and variables. The results indicate that hydraulic fracturing is an effective guarantee of high-production CBM wells in the first several months during a high-rank CBM field development. However, the effect of hydraulic fracturing on enhancing the gas production of CBM wells decreases with time because the initial reservoir permeability, lower than the hydraulic fracture permeability, limits the adsorption, diffusion and flow of CBM. This limitation inevitably leads to a slow gas production rate when the adsorbed CBM from the initial reservoir becomes the main gas source instead of the fracturing-affected zone. Gas content and permeability are two key factors that dominate CBM well productivity, because they perform elementary roles in controlling the volume of gas sources and conductivity, respectively. The structural setting and hydrogeological condition are also two important factors that dominate CBM well productivity because they can influence the spatial distribution of permeability and gas content as well as other factors (such as aquifers).

13/00740 Seawater biodegradation of alkanolamines used for CO_2-capture from natural gas

Brakstad, O. G. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 271–277.

Alkanolamines used for CO_2-capture in natural gas (NG) may be released to the marine environment from coastal and offshore NG facilities. In this study biodegradation of alkanolamines in seawater was investigated. Screening of 20 alkanolamine candidates for ultimate biodegradability showed that biodegradation rates followed the order primary = secondary > tertiary > sterically hindered alkanolamines. Biodegradation studies of monoethanolamine (MEA), diethanolamine (DEA) and methyl-diethanolamine (MDEA) at seawater temperatures of 10–32 °C were performed with respirometric and chemical analyses, showing that temperature-related biodegradation was more pronounced for DEA than for MEA, while MDEA remained recalcitrant at all temperatures. No effect of concentration was detected when DEA and MDEA biodegradation was compared at initial concentrations of 2 and 5 mg/l. PCR-DGGE analyses of bacterial 16S rRNA gene fragments from seawater samples collected during the biodegradation experiments at 20 °C revealed one major band associated with DEA biodegradation. Analyses of the 16S rRNA gene fragments by cloning and sequencing showed predominance of the class *Alphaproteobacteria* in all samples, but biodegradation of DEA at 20 °C resulted in an increased fraction of *Gammaproteobacteria*. Sequence analyses of cloned inserts were performed after suppressive subtraction hybridization (SSH) cDNA PCR amplification of genes expressed during growth of the strain *Pseudomonas* sp. P6 on the alkanolamine 1-aminopropan-2-ol. The results of these analyses indicated that gene expression was associated with cobalamine (vitamin B_{12}) synthesis with 1-aminopropan-2-ol incorporation in the vitamin B_{12} complex, and with putative enzymes involved in the glyoxylate and tricarboxylic acid cycles. In addition, the results suggested a general up-regulation of transcriptional and translational activities, including amino acid metabolism.

13/00741 The influence of gas storage parameters on gas emission rate from borehole

Gao, J. and Shang, B. *Safety Science*, 2012, 50, (4), 869–872.

Gas emission rate from borehole is one of the most important indexes for the coal and gas outburst prediction. The mathematical model of gas flow in the coal seam, gas flow into the measuring chamber, gas pressure change in the measuring chamber, and gas flow out of the chamber through the pipe is established. Gas migration in the coal seam, gas pressure in borehole chamber and gas flow in pipe is simulated using the finite difference method. Gas emission rate is obtained under dynamic boundary conditions. The influence of gas storage parameters on gas emission rate from borehole is analysed. Results show that: the gas pressure and the permeability coefficient have great impacts on the value of gas flow quantity in borehole. The larger the original gas pressure of coal seam and the permeability coefficient of coal seam are, the greater the maximum value of gas emission rate form borehole and the later the maximum appears.

13/00742 The removal of CO_2 and N_2 from natural gas: a review of conventional and emerging process technologies

Rufford, T. E. *et al. Journal of Petroleum Science and Engineering*, 2012, 94–95, 123–154.

This article provides an overview of conventional and developing gas processing technologies for CO_2 and N_2 removal from natural gas. Process technologies based on absorption, distillation, adsorption, membrane separation and hydrates are considered. For each technology, the authors describe the fundamental separation mechanisms involved and the commonly applied process flow schemes designed to produce pipeline quality gas (typically 2% CO_2, <3% N_2) and gas to feed a cryogenic gas plant (typically 50 ppmv CO_2, 1% N_2). Amine absorption technologies for CO_2 and H_2S removal (acid gas treating) are well established in the natural gas industry. The advantages and disadvantages of the conventional amine- and physical-solvent-based processes for acid gas treating are discussed. The use of CO_2 selective membrane technologies for bulk separation of CO_2 is increasing in the natural gas industry. Novel low-temperature CO_2 removal technologies such as ExxonMobil's Controlled Freeze Zone^{TM} process and rapid cycle pressure swing adsorption processes are also emerging as alternatives to amine scrubbers in certain applications such as for processing high CO_2 concentration gases and for developing remote gas fields. Cryogenic distillation remains the leading N_2 rejection technology for large scale (feed rates greater than 15 MMscfd) natural gas and liquefied natural gas plants. However, technologies based on CH_4 selective absorption and adsorption, as well as N_2 selective pressure swing adsorption technologies, are commercially available for smaller scale gas processing facilities. The review discusses the scope for the development of better performing CO_2 selective membranes, N_2 selective solvents and N_2 selective adsorbents to both improve separation power and the durability of the materials used in novel gas processing technologies.

13/00743 Transportation and storage under a dynamic price cap regulation process

Breton, M. and Kharbach, M. *Energy Economics*, 2012, 34, (4), 918–929.

This paper studies the welfare effects of price cap regulation (PCR) in the gas transportation and storage industry. PCR is one of the preferred mechanisms aimed at protecting consumers from monopolistic behaviour in network industries. This paper models the optimization problem of the regulated company as a bi-level optimization problem, where the demand for transportation and storage access is derived from the oligopolistic equilibrium in the downstream distribution market. This outlines the impact of the capacity constraint on the reaction function of the distribution companies and on the optimal access prices. This is particularly relevant since most long-haul gas pipelines are used at capacity or near capacity. Since price cap weight factors are adjusted yearly on the basis of the revenue of the regulated company, the impact of PCR is on the access prices, marketed quantities, industry profits and consumer welfare is analysed in a dynamic setting. The study considers both the case where prices are set myopically, and the case where the impact of pricing decisions on future weight factors is taken into account by the regulated company. Due to the direct link between the demand for pipeline access and storage, and to the capacity constraints, some results from the literature on PCR do not hold in this case. Indeed, when the capacity constraint is binding, the impact of a price cap is a reduction in consumer surplus, and benefits of the mechanism are essentially captured by the downstream distribution companies. Moreover, it was found that the imposition of a price cap always results in a higher transportation volume, eventually resulting in a binding capacity constraint, and therefore in a decrease in consumer surplus. Examples with representative parameter values are provided where consumer surplus is lower after regulation than before regulation. It was also found that there is no significant advantage for the regulated company to set prices strategically in order to manipulate the price cap constraint. It is worth observing that one of the advantages is the incentives PCR gives companies to increase productivity and reduce costs; this particular effect of PCR is not taken into account in this setting, where productivity and costs are assumed constant over time. The price cap constraint is usually adjusted on a 5-year basis to account for changes in productivity and costs. It is interesting to note that strategic manipulations of the price cap constraint reported in the literature are related to this specific aspect. Notice that the results are derived assuming that the price cap constraint is constant over time to simplify the exposition; however, all results are valid for any price cap value, constant or not, provided that the cap is less than one. One important aspect of the gas industry is the high uncertainty in the demand function. Indeed, demand for gas depends on prices of alternative energy sources and on climatic and economic conditions. Uncertain demand and prices make the storage facilities even more important as a means to allow the exercise of real options to postpone or increase distribution. An interesting extension, left for further research, is the investigation of the impact of demand uncertainty on the value of storage for the distribution firm, and on the pricing decisions of the regulated firm. Since uncertainty in demand makes storage even more appealing, there is no reason why these findings would not be robust, that is, the imposition of a price cap would still increase the demand for storage, and this would ultimately result in a pipeline used at full capacity, a situation where a price cap is no longer welfare enhancing.

13/00744 Well impairment by fines migration in gas fields

Zeinijahromi, A. *et al. Journal of Petroleum Science and Engineering*, 2012, 88–89, 125–135.

Well productivity decline has been widely observed for gas wells producing reservoir fines. The phenomenon has been explained by lifting, migration and subsequent plugging of the pores by the fine particles, finally resulting in permeability decrease. It has been observed in numerous core flood tests and field cases. The new basic equations for the detachment of fine particles, their migration and size exclusion, causing the rock permeability decline during gas production, have been derived. The analytical model developed for the regime of steady state gas production with a gradual accumulation of strained particles, exhibits linear skin factor growth versus the amount of produced reservoir fines. The modelling results are in a good agreement with the well production history.

Economics, business, marketing, policy

13/00745 Gulf of Mexico Gas Hydrate Joint Industry Project Leg II logging-while-drilling data acquisition and analysis

Collett, T. S. *et al. Marine and Petroleum Geology*, 2012, 34, (1), 41–61.

One of the objectives of the Gulf of Mexico Gas Hydrate Joint Industry Project Leg II (GOM JIP Leg II) was the collection of a comprehensive suite of logging-while-drilling (LWD) data within gas-hydrate-bearing sand reservoirs in order to make accurate estimates of the concentration of gas hydrates under various geologic conditions and to understand the geologic controls on the occurrence of gas hydrate at each of the sites drilled during this expedition. The LWD sensors just above the drill bit provided important information on the nature of the sediments and the occurrence of gas hydrate. There has been significant advancements in the use of downhole well-logging tools to acquire detailed information on the occurrence of gas hydrate in nature: From using electrical resistivity and acoustic logs to identify gas hydrate occurrences in wells to where wireline and advanced logging-while-drilling tools are routinely used to examine the petrophysical nature of gas hydrate reservoirs and the distribution and concentration of gas hydrates within various complex reservoir systems. Recent integrated sediment coring and well-log studies have confirmed that electrical resistivity and acoustic velocity data can yield accurate gas hydrate saturations in sediment grain supported (isotropic) systems such as sand reservoirs, but more advanced log analysis models are required to characterize gas hydrate in fractured (anisotropic) reservoir systems. In support of the GOM JIP Leg II effort, well-log data montages have been compiled and presented in this report which includes downhole logs obtained from all seven wells drilled during this expedition with a focus on identifying and characterizing the potential gas-hydrate-bearing sedimentary section in each of the wells. Also presented and reviewed in this report are the gas-hydrate saturation and sediment porosity logs for each of the wells as calculated from available downhole well logs.

13/00746 Hydromethane: a bridge towards the hydrogen economy or an unsustainable promise?

Villante, C. and Genovese, A. *International Journal of Hydrogen Energy*, 2012, 37, (15), 11541–11548.

Pure hydrogen use in spark ignition (SI) ICE requires a dedicated engine design to optimize the high speed flame and the high pressure and temperature inside the combustion chamber. But, on the other end, may lead to high exhaust emissions of nitrogen oxides NO_x. Moreover, hydrogen fuelled vehicles also suffer of a very low mileage due to the very low energy density of the fuel, since hydrogen as a compressed gas at 200 atmospheres and ambient temperature has around 5% of the energy of gasoline of the same volume. All these motivations, together with the now capillary diffusion of natural gas (NG) distribution for residential and transportation purposes (especially in Europe) is making more and more interesting the option of H_2 using as an additive to natural gas: NG powered vehicles, in fact, reached a very high maturity with high reliability and environmental performances. In recent years experimentations were conducted in many laboratories and research centres to verify the positive effects of hydrogen when blended with natural gas. The maturity achieved by H_2–NG mixtures is also stated by commercialized gas which is available in USA with the registered trademark of Hythane® (a mixture of 20% H_2–80% NG in volume). In this paper the hydro-methane option is fully outlined, a complete energy analysis and environmental sustainability is realized, considering all the main possible options available in mixture production and final use.

13/00747 Modularity analysis of the Canadian natural gas sector

Ivanenko, V. *Energy Economics*, 2012, 34, (4), 1196–1207.

The paper describes the technological process presented as a chain of tasks that natural gas companies in Canada perform to move natural gas products from the geological formation to the final consumer. The paper has identified standards common to the chain's segments, or interfaces, and sought to categorize them according to the degree of contract specificity. Consistently with the transaction cost theory, the development of industry-wide norms allows firms to operate at arm's length and, hence, to be less fettered in their choice of clients and suppliers. On the contrary, long-term and client-specific contracts are commonplace in sectors where a high degree of interdependency in the supplier-client pairs is unavoidable due to market imperfections. The study has attempted to rank the segments of the chain in terms of standardization using subjective evaluation. It has concluded that the marketing segment shows the highest degree of standardization, which, theoretically, makes easy establishing cooperative relationship between independent companies. The situation in the other three segments is more complicated. Some of their members cannot coordinate activities using the market instruments alone but are locked in supplier–client pairs. On the top of that, certain market operations, such as the transportation part of local distribution companies, shows their in-built dependence on governmental input raising the question if they should be a part of the public system in the first place. The paper suggests two topics for further research. First, it shows the need for a better indicator of structural dependency in supplier–client pairs than the subjective evaluation of contract specificity. One alternative, explored in an earlier study, would be to use the number of firm's suppliers or clients as an inverse indicator of firm's dependency on its partners. In this interpretation, the degree of diversification acquires additional meaning. Apart from being an insurance against potential chain breakdowns, it becomes a measure of status that the firm attains within the chain. Another potentially useful indicator is the share of risk that each partner accepts in joint business projects. Assuming the decreasing absolute risk aversion in wealth, wealthier firms are more likely to take the risk from business partners more constraint in resources. In this case, the larger is the firm, the higher should be its hierarchical status within the supplier–client pairs.

13/00748 Optimal path for China's strategic petroleum reserve: a dynamic programming analysis

Bai, Y. *et al. Energy Economics*, 2012, 34, (4), 1058–1063.

This paper proposes a dynamic programming model to explore the optimal stockpiling path for China's strategic petroleum reserve before 2020. The optimal oil acquisition sizes in 2008–2020 under different scenarios are estimated. The effects of oil price, risks and elasticity value on inventory size are further investigated. It is found that the optimal stockpile acquisition strategies are mainly determined by oil price and total inventory costs. While oil supply disruption is not considered, China's optimal stockpile acquisition rate increases from 19.2 to 52 million barrels from 2008 to 2020. If an oil supply disruption occurs, the oil acquisition rate will be reduced significantly. However, it may not be a good strategy to interrupt oil reserve activities in order to minimize the total costs for the entire planning period.

13/00749 Review of progress in evaluating gas hydrate drilling hazards

McConnell, D. R. *et al. Marine and Petroleum Geology*, 2012, 34, (1), 209–223.

Shallow drilling hazard assessment consists of geological/geophysical review of drill sites to enable the avoidance or effective mitigation of problems that can affect the safe drilling of the 'top-hole' section of wells. Primary seafloor hazards include infrastructure, hardgrounds, chemosynthetic communities, and areas of high slope or potential seafloor instability. Shallow subsurface hazards include strata that may contain overpressured water, free gas, or gas hydrate. Among these issues, the potential hazards posed by gas hydrate have historically been the most difficult to quantify and constrain. This paper reviews the history of gas hydrate shallow hazard assessment, much of which has been framed by difficulties in remote detection and quantification of typical low-saturation, mud-hosted hydrate occurrences. Recent drilling results indicate that such accumulations can be safely drilled using existing industry protocols. However, assessment of drilling hazards associated with high saturation, sand-hosted hydrates warrant further investigation, and therefore was a key focus of the Gulf of Mexico Gas Hydrate Joint Industry Project Leg II (JIP Leg II) program conducted in 2009. Pre-drill site hazard assessment for JIP Leg II utilized standard industry methods in which geohazards associated with gas hydrate and free gas were identified in a primarily-qualitative manner using seismic amplitude analysis, seismic stratigraphic interpretation, and geo-pressure analysis. While these methods can reliably detect shallow hydrocarbons, including highly-concentrated gas hydrates, they are not sufficient to determine if free gas may exist below gas hydrate, particularly where they occur in close vertical succession. Such undetected free gas occurrences can pose potential drilling hazards that can be quantitatively assessed using advanced seismic methods.

13/00750 Risk analysis for oil & gas pipelines: a sustainability assessment approach using fuzzy based bow-tie analysis

Shahriar, A. *et al. Journal of Loss Prevention in the Process Industries*, 2012, 25, (3), 505–523.

Vast amounts of oil and gas (O&G) are consumed around the world every day that are mainly transported and distributed through pipelines. In Canada, the total length of O&G pipelines is approximately 100,000 km, which is the third largest in the world. The integrity of these pipelines is of primary interest to O&G companies, consultants, governmental agencies, consumers and other stakeholders due to adverse consequences and heavy financial losses in case of systems failure. Fault tree analysis (FTA) and event tree analysis (ETA) are two graphical techniques used to perform risk analysis, where FTA represents causes (likelihood) and ETA represents consequences of a failure event. 'Bow-tie' is an approach that integrates a fault tree (on the left side) and an event tree (on the right side) to represent causes, threat (hazards) and consequences in a common platform. The traditional 'bow-tie' approach is not able to characterize model uncertainty that arises due to assumption of independence among different risk events. In this paper, in order to deal with vagueness of the data, the fuzzy logic is employed to derive fuzzy probabilities of basic events in fault tree and to estimate fuzzy probabilities of output event consequences. The study also explores how interdependencies among various factors might influence analysis results and introduces 'fuzzy utility value' to perform risk assessment for natural gas pipelines using triple bottom line sustainability criteria, namely, social, environmental and economic consequences. The present study aims to help owners of transmission and distribution pipeline companies in risk management and decision-making to consider multi-dimensional consequences that may arise from pipeline failures. The research results can help professionals to decide whether and where to take preventive or corrective actions and help informed decision-making in the risk management process. A simple example is used to demonstrate the proposed approach.

13/00751 SPHERA project: assessing the use of syngas fuels in gas turbines and combined cycles from a global perspective

Chacartegui, R. *et al. Fuel Processing Technology*, 2012, 103, 134–145.

The differential aspects derived from burning syngas fuels in a conventional combined cycle power plant were explored in the SPHERA project, covering very different aspects of the power plant like performance, analysis, turbomachinery design, heat transfer and integrity issues. This work was organized in two stages: analysis of syngas operation for the current technology and development/suggestion of modifications to fully optimize the operation on syngases. These activities were scheduled in six tasks, each concentrated on a particular topic. Modern gas turbines, and therefore combined cycle power plants, cannot run efficiently on low BTU syngas fuels without the necessary technology update (this is, strictly speaking, not true since syngas fuels can be used though at the expense of a dramatic derating of the engine; this is why the text indicates ‘efficiently’, so as to highlight the loss in efficiency experienced by derated engines). Thus, the development of specific components for this type of operation is therefore deemed necessary. Some of these components that need major revisions are: combustors (flame stability, emissions, reliability), Task II; sirst high-pressure turbine stage (aerodynamic design and size), Tasks III and V; turbine cooling systems (especially the high pressure section), Task IV. If the gas turbine is integrated in a combined cycle, the bottoming system has to be scaled-up in accordance (heat recovery steam generator, steam turbine and condenser) since the gas turbine exhaust mass flow increases by around 15–20%; if this surplus mass flow is not bypassed in the steam generator, the power output of the bottoming system should increase accordingly (Task V). Even though in the case of bypassing part of the exhaust flow from the topping system there would no need for a new design, part of the potential of the new cycle would be lost. In the case where no flow is bypassed, the main bottlenecks found in the steam cycle are related to the maximum capacity of the electric generator, condenser and other auxiliary equipment. In this regard, updating some of the systems is economically feasible (for instance, fin fan cooler or feedwater pumps) whereas in other cases it is advisable to alter the original operating conditions (for instance the condenser pressure). In some instances, substituting the equipment is compulsory; this is the case of the electric generator. The recommended modifications and updates to adapt combined cycles to syngas operation have been summarized into three different levels of priority. They were derived from the multiple analyses developed along this project and they can be regarded as a global roadmap seeking to adapt combined cycles to syngas operation considering current technically feasible and economically competitive modifications only.

13/00752 Weight-of-evidence environmental risk assessment of dumped chemical weapons after WWII along the Nord-Stream gas pipeline in the Bornholm Deep

Sanderson, H. *et al. Journal of Hazardous Materials*, 2012, 215–216, 217–226.

In connection with installation of two natural gas pipelines through the Baltic Sea between Russia and Germany, there has been concern regarding potential re-suspension of historically dumped chemical warfare agents (CWA) in a nearby dump site and the potential environmental risks associated. One hundred and ninety-two sediment and 11 porewater samples were analysed for CWA residues, both parent and metabolites in 2008 and 2010 along the pipeline corridor next to the dump site. Macrozoobenthos and background variables were also collected and compared to the observed CWA levels and predicted potential risks. Detection frequencies and levels of intact CWA found were low, whereas CWA metabolites were more frequently found. Re-suspension of CWA residue-containing sediment from installation of the pipelines contributes marginally to the overall background CWA residue exposure and risk along the pipeline route. The multivariate weight-of-evidence analysis showed that physical and background parameters of the sediment were of higher importance for the biota than observed CWA levels.

Derived gaseous fuels

13/00753 Gasification of rice straw in a fluidized-bed gasifier for syngas application in close-coupled boiler-gasifier systems

Calvo, L. F. *et al. Bioresource Technology*, 2012, 109, 206–214.

The feasibility and operation performance of the gasification of rice straw in an atmospheric fluidized-bed gasifier was studied. The gasification was carried out between 700 and 850 °C. The stoichiometric air–fuel ratio (A/F) for rice straw was 4.28 and air supplied was 7–25% of that necessary for stoichiometric combustion. Mass and power balances, tar concentration, produced gas composition, gas phase ammonia, chloride and potassium concentrations, agglomeration tendencies and gas efficiencies were assessed. Agglomeration was avoided by replacing the normal alumina-silicate bed by a mixture of alumina-silicate sand and MgO. It was shown that it is possible to produce high quality syngas from the gasification of rice straw. Under the experimental conditions used, the higher heating value (HHV) of the produced gas reached 5.1 MJ N m^{-3}, the hot gas efficiency 61% and the cold gas efficiency 52%. The obtained results prove that rice straw may be used as fuel for close-coupled boiler-gasifier systems.

13/00754 High-pressure hydrogen/carbon monoxide syngas turbulent burning velocities measured at constant turbulent Reynolds numbers

Chiu, C. W. *et al. International Journal of Hydrogen Energy*, 2012, 37, (14), 10935–10946.

Using a double-chamber explosion facility, the authors measure high-pressure turbulent burning velocities (S_T) of lean syngas (35%H_2/65%CO) spherical flames at constant turbulent Reynolds numbers ($Re_T \equiv u'L_I/\nu$) varying from 6700 to 14,200, where the root-mean-square turbulent fluctuation velocity (u') and the integral length scale (L_I) are adjusted in proportion to the decreasing kinematic viscosity of reactants ν) at elevated pressure (p) up to 1.2 MPa. Results show that, contrary to popular scenario for turbulent flames, at constant Re_T, S_T decreases similarly as laminar burning velocities (S_L) with increasing p in minus exponential manners. Moreover, at constant p, S_T/S_L increases noticeably with increasing Re_T. It is found that the present very scattering S_T/S_L data at different p and Re_T can be nicely merged onto a relation of $S_T/u' = 0.49Da^{0.25}$, where Da is the turbulent Damköhler number and values of S_T/u' tends to level-off when $Da > 160$ and $p > 0.7$ MPa.

13/00755 Initiating methanogenesis of vegetable waste at low inoculum-to-substrate ratio: importance of spatial separation

Lü, F. *et al. Bioresource Technology*, 2012, 105, 169–173.

With the goal of starting-up the methanogenesis of easily biodegradable waste with minimum inoculum, the present work evaluated different inoculum-to-substrate ratios ($r_{I/S}$) in completely mixed systems and in the systems with spatial separation of inoculum and waste. It was found difficult to initiate methanogenesis in the completely mixed systems, even at high $r_{I/S}$ 1.105 on a volatile solid basis. Fermentation efficiencies were independent of $r_{I/S}$. In the spatial-separation systems with a low total $r_{I/S}$ 0.053, the ultimate methane yield (35 °C, 1 atm) reached 445 mL/g-VS added for the inoculum-waste initially completely separated system. The yields decreased to 285, 181, and 34 mL/g-VS added, respectively, for partially separated systems with the ratios controlled at 1.105, 0.254, and 0.113 in the inoculum-containing reactors. This demonstrates the importance of setting spatial separation between inoculum and waste when inoculation is employed. An appropriate inoculation method would initiate methanogenesis rapidly even at low inoculum-to-substrate ratios.

13/00756 Microbial production of methane and carbon dioxide from lignite, bituminous coal, and coal waste materials

Opara, A. *et al. International Journal of Coal Geology*, 2012, 96–97, 1–8.

The aim of this study was to examine microbial methane and CO_2 production from bituminous coal waste, lignite, and bituminous coal materials. Bituminous coal and coal waste material were obtained from a Utah mine and lignite was obtained from a commercially available North Dakota sample. Microbial populations were cultured from hydrocarbon-rich environments and locations where natural methanogenesis was occurring. Various pulverized coal and coal waste materials were combined with selected microbial inocula and different types and levels of nutrient amendments. After a 30-day reaction period at about 23 °C, headspace methane and CO_2 were analysed using gas chromatography. With increasing nutrient concentrations (0, 10 and 50%), coal waste generated an extrapolated equivalent of 36, 53 and 16,000 scf of CH_4/ton/year and 1870, 4400 and 8000 scf of CO_2/ton/year. Methane produced from native and nutrient-amended bituminous coal waste materials was the same order of magnitude as that produced from bituminous coal but lower than that produced from lignite. CO_2 generation from coal waste materials, with no nutrient addition was over twice as high as that produced from analogous bituminous coal. The results of this study suggest that coal waste products can be converted to useful fuel at volumes that may be commercially viable.

13/00757 Modeling and simulation of catalytic partial oxidation of methane to synthesis gas by using a plasma-assisted gliding arc reactor

Rafiq, M. H. *et al. Fuel Processing Technology*, 2012, 101, 44–57.

In this study, a numerical investigation of the catalytic partial oxidation (CPO) of methane to synthesis gas (syngas) using a gliding arc (GlidArc) reactor is presented. A two-dimensional heterogeneous plug-flow model with radial dispersion and no gradients inside the catalyst pellet are used, including the transport equations for the gas and solid phase and reaction rate equations. The governing equations of this model formed a set of stationary differential algebraic equations coupled with the non-linear algebraic equations, and were solved numerically using in-house MATLAB code. Model results of CPO of methane were compared to previous experimental data with the GlidArc reactor found in the literature. A close match between the calculated and experimental results for temperature, reactant (CH_4 and O_2) conversion, H_2 and CO yields and species mole-fraction was obtained. The developed model was extended to predict and quantify the influence of the gas hour space velocity (GHSV) as well as determine the influence of the reactor energy density (RED), the O_2/

CH_4 molar ratio and the O_2/N_2 molar ratio. The predicted behaviours for the species mole-fraction, reactants conversion, H_2 and CO yields and temperature along the length of the reactor have been analysed.

13/00758 Modification effect of natural mixed rare earths on Co/γ-Al_2O_3 catalysts for CH_4/CO_2 reforming to synthesis gas

Zeng, S. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 9994–10001.

The study first investigated the modification effect of natural mixed rare earths (MRE) on cobalt catalysts for CH_4/CO_2 reforming to synthesis gas. The Co/γ-Al_2O_3 catalysts modified with the natural mixed rare earths were synthesized by the impregnation method, and characterized via ICP, BET, XRD, H_2-TPR, TEM and TG–DSC techniques. The result showed that the addition of mixed rare earths enhanced the anti-sintering ability of metallic cobalt after reduction and improved anti-coke performance of the catalysts via the synergic effect of mixed rare earths. The 20% Co/γ-Al_2O_3 catalyst promoted by the appropriate natural mixed rare earths exhibited good activity and stability with low carbon formation at 800 °C for 320 h reaction.

13/00759 On the effects of running existing combined cycle power plants on syngas fuel

Chacartegui, R. *et al. Fuel Processing Technology*, 2012, 103, 97–109.

The use of gasified fuels for electricity production is of increasing interest as an alternative to traditional fuels especially in regions with abundant biomass or coal resources. Nevertheless, its use in current gas turbine technologies is challenging due to the differences in fuel composition with respect to conventional natural gas. In this paper, the effects of using a set of syngas fuels on the components of a reference combined cycle are studied. The analyses shown in this paper are focused on the expansion of the different combustion products through the turbine and on the bottoming cycle. In the gas turbine, the effect of the different combustion product properties and mass flows on the performance of the expansion process is studied first. Then the impact on the turbine cooling system of a standard natural gas engine is analysed. In the bottoming cycle the higher load on each particular component is studied aiming to find bottlenecks to the operation under the new operating conditions. The results show that from the combined cycle power plant standpoint, excluding the gasification island, an adequate upgrade of the components of the power block results in a combined cycle performance in syngas operation that is similar to using natural gas. This provides the combined cycle owner/operator with a valuable perspective to evaluate technology risks and appraise potential retrofitting of their plants depending on fuel cost and availability.

13/00760 Reforming of a model biogas on Ni and Rh–Ni catalysts: effect of adding La

Lucrédio, A. F. *et al. Fuel Processing Technology*, 2012, 102, 124–131.

Ni catalysts supported on γ–Al_2O_3 modified by Rh and La were prepared and evaluated on the reforming of a model biogas. The catalysts were characterized by EDS, XRD, TPR, XANES and surface area estimation (BET). The results showed that in the original Ni catalyst, the Ni interacted strongly with the alumina support, exhibiting high reduction temperatures in TPR tests. In the catalytic tests, the addition of Rh on Ni catalysts improved CH_4 conversion but also increased carbon deposition, possible by causing the segregation of Ni species under the reaction conditions. The presence of La on Ni catalysts reduced the carbon deposition by favouring the gasification of carbon species. Addition of synthetic air to the process improved the CH_4 conversion and also decreased the carbon formation. The catalysts Ni, Rh–NiLa, and Rh showed good results in the conversion of model sulfur-free biogas, which suggests that they are promising catalysts to be tested in conversion of real biogas.

LNG

13/00761 Approach enhancing inherent safety application in onshore LNG plant design

Tanabe, M. and Miyake, A. *Journal of Loss Prevention in the Process Industries*, 2012, 25, (5), 809–819.

This study aims to provide the approach for inherent safety design of onshore liquefied natural gas (LNG) plants to be applied at the very early stages (concept definition phase) of the project development. Onshore LNG plant development project starts from the ‘concept definition’ phase, where financial feasibility is estimated and major conditions, such as site location and plant foot print, are set. The inherent safety design basic criteria and design measures should be identified and selected when setting the basic conditions during the Concept Definition phase of the project development, such as the site location (relative location from populated areas), site condition (prevailing wind direction) and plant production capacity (number of process train, number of product tanks). The safety measures, which are usually not fully developed at the project early stages in the current design execution practices, are the emergency systems, which mitigate an accident escalation, the modularized plant and layout, and the tank selection. The inherent safety design measures discusses in this paper were identified based on the categories of plot plan, emergency system, and module plant application. The proposed approach will contribute to improve inherent safety design of onshore LNG plants and it will also yield schedule and cost benefits.

13/00762 Development of a synthesis tool for gas-to-liquid complexes

Ellepola, J. *et al. Computers & Chemical Engineering*, 2012, 42, 2–14.

Optimal synthesis of a gas-to-liquid (GTL) complex is complicated due to many degrees of freedom in a highly constrained design space. One can choose between alternative, competing syngas manufacturing technologies, different types of Fischer–Tropsch catalysts and reactors, with numerous connectivity options and a range of operational conditions. On the other hand, the design space is confined by equipment, operational and knowledge constraints. Furthermore, economic performance needs to be aligned with carbon and energy efficiencies. To support GTL process design, a computational synthesis tool is under development. Its purpose is to find and analyse the optimum structure and operational conditions for a given market scenario. The process model covers alternative syngas generation units and Fischer–Tropsch reactors with an extensive syngas recycle structure. The process units interact with the utility system, where power can be generated from off-gas and/or excess steam. The units are modelled in a reduced, input–output way by algebraic equations, reflecting mass and energy balances and pressure effects. A superstructure arises when considering multiple stages for Fischer–Tropsch synthesis with parallel reactors. The synthesis tool, implemented in AIMMS®, is applied to a realistic sample problem, showing profit optimization by varying the distribution of NG to syngas generation units with different efficiencies. A sensitivity analysis is carried out by means of singular value decomposition of sensitivity matrices to find dominant patterns of parametric influence on the optimum.

13/00763 Energy consumption reduction in CO_2 capturing and sequestration of an LNG plant through process integration and waste heat utilization

Alabdulkarem, A. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 215–228.

Liquefied natural gas (LNG) plants are energy intensive. As a result, the power plants operating these LNG plants emit high amounts of CO_2. To mitigate global warming that is caused by the increase in atmospheric CO_2, CO_2 capture and sequestration (CCS) using amine absorption is proposed. However, the major challenge of implementing this CCS system is the associated power requirement, increasing energy consumption by about 15–20%. In order to reduce such energy consumption, innovative process integration and waste heat utilization is proposed. Four waste heat sources and six potential uses were uncovered. A new integrated CCS configuration is proposed, which integrates the APCI LNG plant and the driver cycle with the CCS plant. HYSYS simulation software was used to simulate the CO_2 capture cycle using monoethanolamine solvent, natural gas combined cycles, CO_2 compression cycle and CO_2 liquefaction cycles. The developed models were validated against experimental data from the literature with good agreement. Net available power enhancement in one of the proposed CCS configuration is 26.3 MW, which is 16.31% more than the conventional CCS configuration. Pinch analysis method was used to compare the utility cooling and utility heating of the proposed and conventional CCS configurations. The result of the pinch analysis shows that the proposed CCS configuration requires 23.86% less utility cooling than the conventional CCS configuration.

13/00764 Experimental approach to suppress two-phase flow in cryogenic liquid transfer process with the inverted U-bend pipe

Baek, S. and Jeong, S. *Experimental Thermal and Fluid Science*, 2012, 42, 116–124.

The liquefied natural gas (LNG) offloading process from LNG cargo to storage tank includes substantial vertical upward fluid transportation. During this LNG transportation process, local boiling may occur at elevated position of the transport pipe due to the decrease of hydrostatic pressure and obstruct liquid flow, concluding long transport time or insufficient transport to a tank. Small-scale LN_2 (liquid nitrogen) transfer system has been fabricated to simulate this LNG transportation process and flow characteristics. Subcooled LN_2 is transferred to 5 m upward, 1 m horizontally, and 5 m downward through vacuum insulated stainless steel pipe. Glass pipes are installed at the middle part of transportation pipes to visualize the two-phase flow pattern during fluid transfer. Cryogenic valve is installed at the outlet of transfer pipe to regulate the system pressure inside the transfer tube. Pressurization by manipulating the cryogenic valve at the outlet, effectively suppressed two-phase flow, which resulted in transportation advantages, such as low pressure drop and smooth flow. This paper presents the detailed experimental data of the whole procedure of the tested LN_2 transfer system.

13/00765 Performance enhancement of propane pre-cooled mixed refrigerant LNG plant

Mortazavi, A. *et al. Applied Energy*, 2012, 93, 125–131.

Liquefied natural gas (LNG) and chemical processing are energy-intensive facilities, such that any enhancement of their efficiency will result in abundant reduction of energy consumption and greenhouse gas emissions. To enhance LNG plant energy efficiency, the potential of various options for improving liquefaction cycle efficiency is investigated in this study. After developing models for the LNG process using ASPEN software, four expansion loss recovery options are simulated. The simulation results show that the compressor power reduction, expansion work recovery and LNG production increase can be achieved as much as 2.68 MW, 3.82 MW and 1.24%, respectively, by replacing conventional expansion processes with expanders. By implementing all of the enhancements, the power consumption per unit mass of LNG could be reduced by 7.07% and 3.68%, with and without considering deduction of the recovered power from the total required power, respectively. Therefore, the expansion work recovery is an important option to be implemented in LNG plants.

Hydrogen generation and storage

13/00766 Characterization and the hydrogen storage capacity of titania-coated electrospun boron nitride nanofibers

Shahgaldi, S. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11237–11243.

In the present work, titania-coated (TiO_2) boron nitride nanofibres were produced by the electrospinning method, and the effect of heat treatment on the nanofibres was studied. Electrospinning method is often adopted for the synthesis of one-dimensional nanofibres due to high productivity, simplicity, and cost-effectiveness. In this study, boric oxide was deposited on co-electrospun polyacrylonitrile and TiO_2. TiO_2-coated boron nitride nanofibres, with a diameter of 100 nm, were obtained after heat treatment and nitridation. The effects of heat treatment on the morphology, surface area and hydrogen storage capacity were studied extensively. Scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), and transmission electron microscopy (TEM) showed long, bead-free nanofibres and the presence of TiO_2 nanoparticles on the nanofibres. X-ray diffraction (XRD) and Fourier transform infrared (FTIR) spectroscopy depicted hexagonal structures of boron nitride. The hydrogen uptake capacities of the nanofibres were investigated by pressure composition isotherm (PCI) in the pressure range of 1–70 bar at room temperature.

13/00767 Continuous hydrogen production by sorption enhanced steam methane reforming (SE-SMR) in a circulating fluidized bed reactor: sorbent to catalyst ratio dependencies

Arstad, B. *et al. Chemical Engineering Journal*, 2012, 189–190, 413–421.

Continuous hydrogen production by sorption enhanced steam methane reforming (SE-SMR) has been studied using a circulating fluidized bed reactor with calcined natural dolomite as CO_2 sorbent and $Ni/NiAl_2O_4$ as catalyst. A steam to methane ratio of 4 was used at 575 °C and ambient pressure. Two experiments, each run for 8 h, were carried out using two different volumetric catalyst to sorbent ratios; 20/80 (experiment A) and 50/50 (experiment B) respectively. In experiment A, run at lower than equilibrium conversion, an initial high conversion that dropped significantly after a few hours was observed, while in experiment B, a stable performance throughout the 8 h time-on-stream close to equilibrium conversion of methane was observed. The experiments show that a circulating fluidized bed reactor configuration is suited for SE-SMR for extended time of operation. The sorbent and catalyst materials used appear to have quite good mechanical properties at the time scale used (8 h), but only a fraction of the sorbent's CO_2 capacity appears to be in use.

13/00768 Electro-extractive fermentation for efficient biohydrogen production

Redwood, M. D. *et al. Bioresource Technology*, 2012, 107, 166–174.

Electrodialysis, an electrochemical membrane technique, was found to prolong and enhance the production of biohydrogen and purified organic acids via the anaerobic fermentation of glucose by *Escherichia coli*. Through the design of a model electrodialysis medium using cationic buffer, pH was precisely controlled electrokinetically, i.e. by the regulated extraction of acidic products with coulombic efficiencies of organic acid recovery in the range 50–70% maintained over continuous 30-day experiments. Contrary to previous reports, *E. coli* produced H_2 after aerobic growth in minimal medium without inducers and with a mixture of organic acids dominated by butyrate. The selective separation of organic acids from fermentation provides a potential nitrogen-free carbon source for further biohydrogen production in a parallel photofermentation. A parallel study incorporated this fermentation system into an integrated biohydrogen refinery for the conversion of organic waste to hydrogen and energy.

13/00769 High-purity hydrogen production through sorption enhanced water gas shift reaction using K_2CO_3-promoted hydrotalcite

Jang, H. M. *et al. Chemical Engineering Science*, 2012, 73, 431–438.

Sorption enhanced water gas shift (SEWGS) reaction is a process concept, which simultaneously carries out the gas phase water gas shift (WGS) reaction ($CO+H_2O \leftrightarrow CO_2+H_2$) and selective chemisorption of the byproduct CO_2 from the gas phase reaction zone for direct production of essentially pure H_2 in a single unit operation. A packed bed sorber-reactor containing an admixture of a WGS catalyst and a CO_2 chermisorbent is used in the process. The concept circumvents the thermodynamic limitation of the WGS reaction and enhances the rate of reaction for H_2 production. In this study, the SEWGS reaction concept was successfully demonstrated by both experiment and numerical simulation using K_2CO_3-promoted hydrotalcite as the CO_2 sorbent. Numerical model simulations were also carried out to investigate the effects of various operating conditions of SEWGS reaction on the process performance. In general, higher H_2O/CO feed ratio, higher fraction of sorbent (chemisorbent ratio in the sorber-reactor), and lower operating temperature favour both H_2 productivity and CO conversion. Higher reaction pressure increases H_2 productivity but decreases CO conversion.

13/00770 Hydrogen production by catalytic cracking of rice husk over Fe_2O_3/γ-Al_2O_3 catalyst

Xu, X. *et al. Renewable Energy*, 2012, 41, 23–28.

Fe_2O_3/γ–Al_2O_3 catalyst is prepared by incipient wetness impregnation. The catalyst is characterized by temperature programmed reduction (TPR), X-ray diffraction (XRD), scanning electron microscope (SEM) and thermogravimetric analysis (TGA). The catalytic activity of Fe_2O_3/γ–Al_2O_3 catalysts is evaluated via the experimental study on the catalytic cracking of rice husk to produce hydrogen in a self-made biomass continuous pyrolysis system. The results show that the reaction activities of the catalysts are greatly influenced by the calcinations temperature for catalyst, the secondary catalytic pyrolysis temperature and the mass ratio of Fe to Al. When the calcinations temperature is 550 °C, the pyrolysis temperature is 500 °C, the secondary catalytic pyrolysis temperature is 700 °C, and the Fe to Al mass ratio is 0.07, the experimental results indicate that Fe_2O_3/γ–Al_2O_3 catalyst could fully convert the volatile matters from biomass pyrolysis into small molecular gases such as H_2, CH_4, CO, CO_2, C_2H_4 and C_2H_6. Meanwhile, the catalyst has shown fine catalytic activity and stability as well as good resistance to coke deposition.

13/00771 Hydrogen production for fuel cells via steam reforming of dimethyl ether over commercial $Cu/ZnO/Al_2O_3$ and zeolite

Li, J. *et al. Chemical Engineering Journal*, 2012, 187, 299–305.

The steam reforming of dimethyl ether (DME) over physical mixture of commercial $Cu/ZnO/Al_2O_3$ and zeolite (HZSM-5 or HUSY) was extensively studied for the hydrogen production for low-temperature fuel cells. Results indicate that time-on-stream DME conversion, hydrogen yield, and selectivity of carbon-containing products were strongly dependent on the zeolites type and mixing method of the hybrid catalyst. Significantly, the powdery mixture of HUSY and $Cu/ZnO/Al_2O_3$ showed much higher and more stable DME conversion and hydrogen yield than the granular mixture with the same composition. However, when substituting HUSY with HZSM-5 ($SiO_2/Al_2O_3 = 38$), almost the same results were obtained irrespective of the mixing methods. These quite different results were explained based mainly on the acidic properties of the zeolites in combination with the two-step reaction mechanism of the titled reaction. The effect of the types of $Cu/ZnO/Al_2O_3$ and zeolites, weight ratio of $Cu/ZnO/Al_2O_3$ to zeolite, and space velocity on the catalytic performance was quantitatively evaluated. Under optimized conditions, over 80% hydrogen yield was achieved at 100% DME conversion, indicating that commercial catalysts are able to give satisfied results. A scheme for hydrogen production for by burning some unconverted DME outside of the reactor to maintain reaction temperature was proposed and the heat balancing indicated that the steam reforming of DME is very promising to supply hydrogen for fuel cells.

13/00772 Hydrogen production from the steam reforming of bio-butanol over novel supported Co-based bimetallic catalysts

Cai, W. *et al. Bioresource Technology*, 2012, 107, 482–486.
This paper reports the hydrogen production through the steam reforming of a bioresource-derived butanol mixture (butanol:acetone: ethanol = 6:3:1 mass ratio) over supported cobalt-based catalysts. The support plays an important role for the catalytic behaviour and Co/ZnO exhibits the best catalytic performance compared to Co/TiO_2 and Co/CeO_2. Moreover, a higher hydrogen yield is obtained over bimetallic Co–Ir/ZnO, which shows an increase in H_2 selectivity and a decrease in CH_4 selectivity under steam reforming conditions, compared to Co/ZnO. Raman results of the used catalysts indicate that the addition of Ir could prevent the coke formation to prolong the catalyst stability.

13/00773 Investigation of hydrogen production in a circulating fast fluidized bed reactor using numerical simulations

Abashar, M. E. E. *Fuel Processing Technology*, 2012, 102, 73–84.
Oxidative reforming of methane for efficient production of hydrogen in a circulating fast fluidized bed reactor (CFFBR) at low pressure and oxygen distribution has been simulated and evaluated. It has been found that the oxidative reforming of methane is inexpensive alternative route to the conventional steam reforming of methane processes. Also, the potential application of *in situ* heat integration in the CFFBR is very promising for energy savings. A comparison between co-feed and oxygen distribution configurations is investigated. The performance of the CFFBR with co-feed configuration is profoundly affected by the development of hot spot temperatures along the length of the reactor. The distribution of oxygen mitigates the temperature along the length of the reactor and eliminates the development of hot spot temperatures and reactor thermal runaway. The results show that the combination of oxygen distribution with part of oxygen directly fed into the reactor is efficient configuration for production of hydrogen and produces almost 100% conversion of methane and high yield of hydrogen up to 2.351 at 70% of the dimensionless reactor length. The sensitivity analysis shows that careful selection of the operation conditions is necessary for best reactor performance.

13/00774 Steam reforming of glycerol over Ni supported alumina xerogel for hydrogen production

Ebshish, A. *et al. Energy Procedia*, 2012, 18, 552–559.
Momentous amount of glycerol is produced as a by-product during biodiesel production by the transesterification of vegetable oils, which are available at low cost in large supply from renewable raw materials. As hydrogen is a clean energy carrier, conversion of glycerol to hydrogen is one among the most attractive ways to make use of glycerol. In this study, the catalytic production of hydrogen by steam reforming of glycerol has been experimentally performed in a fixed-bed reactor. The performance of this process was evaluated over 10 wt% Ni-supported alumina xerogel catalysts. Ni is impregnated over alumina xerogel which was pretreated at different temperatures of 700, 800, 900 and 1000°C. For a comparative purpose, the steam reforming experiments were conducted under same operating conditions, i.e. reaction temperature of 600°C, atmospheric pressure and 1:6 glycerol to water molar ratio where 100% glycerol conversion was obtained in all the runs. The results showed that the hydrogen production increased with the increase in the treatment temperature of the support. The highest amount of hydrogen produced was attained over 10 wt% Ni-doped alumina xerogel pretreated at 1000°C. The catalytic enhancement over the best catalyst system is due to the thermal stability of the support which is treated at highest temperature. Sol gel method of preparation is implemented in the support development and different catalyst systems used in the reforming process were characterized using X-ray powder diffraction, BET surface area and SEM analysis.

13/00775 Sulfur trioxide electrolysis studies: implications for the sulfur–iodine thermochemical cycle for hydrogen production

Mawdsley, J. R. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11004–11011.
This paper describes the efforts to develop a sulfur trioxide (SO_3) electrolyser that could lower the temperature of the SO_3 decomposition step in the sulfur–iodine and hybrid sulfur thermochemical cycles. The objective is to develop an alternative to the standard process of converting SO_3 to SO_2, which is thermal decomposition at 830 °C and above. Thermodynamic calculations show that high SO_3 conversions can be obtained at 590 °C if oxygen is removed during the SO_3 decomposition stage. One way of achieving oxygen removal during SO_3 decomposition is electrolysis, if suitable electrode and electrolyte materials can be found. Active oxygen electrode materials are already developed and the authors have demonstrated suitability of a thin doped-zirconia electrolyte in this study. The main difficulty came in the development of an active and stable SO_3 electrode. Using Ga–V–O/NbB_2/Au electrodes the authors demonstrated high catalytic activity, but could not achieve acceptable electrochemical performance.

04 BY-PRODUCTS RELATED TO FUELS

13/00776 Activated carbon as a catalyst for the synthesis of N-alkylimidazoles and imidazolium ionic liquids

Durán-Valle, C. J. *et al. Catalysis Today*, 2012, 187, (1), 108–114.
An activated carbon Norit RX3 has been treated with acids (sulfuric, nitric and sulfonitric mixture). The modified activated carbons have been characterized by elemental analysis, point of zero charge, N_2 adsorption, XPS and FTIR. The solids obtained have been used as acidic heterogeneous catalyst in the reaction between imidazole and haloalkanes. The reaction with 1-bromobutane yields an ionic liquid, N,N-di-*n*-butyl-imidazolium bromide. Reaction with 2-bromobutane and 1-chlorohexane yields the corresponding N-alkyl-imidazoles. Sulfuric acid treated carbon is the most active catalyst.

13/00777 Effect of relative humidity on the reaction products of alkali activated fly ash

Criado, M. *et al. Journal of the European Ceramic Society*, 2012, 32, (11), 2799–2807.
The alkali activation of fly ash (AAFA) is a chemical process in which the ash is mixed with an alkaline activator and cured at a mild temperature to generate compact solids. Both the curing conditions (temperature, time, relative humidity, etc.) and the nature and concentration of the alkali activator play a key role in the development of the AAFA microstructure and nanostructure, and consequently the properties of these materials. In the present study, fly ash was activated with a 15% water-glass (Na_2SiO_3) + 85% 10-M NaOH solution at 85 °C for 12 h, 7 and 30 days. Two curing methods were used, in which the variable was the relative humidity (RH).

13/00778 Effect of the activation method on the properties and adsorption behavior of bagasse fly ash-based activated carbon

Purnomo, C. W. *et al. Fuel Processing Technology*, 2012, 102, 132–139.
Bagasse fly ash (BFA) has been intensively studied for activated carbon preparation. Several activation methods have been investigated, i.e. physical activation using steam and CO_2, chemical activation using KOH, and one step combination method between chemical and CO_2 physical activation (physiochemical activation). Using coarse BFA particles as the precursor, it was observed that steam activation mainly enhances mesopores, while CO_2 and KOH activation develops particularly the micropores inside the carbon matrix. A typical activation using KOH as the chemical agent at 700 °C improved initial porosity up to 2571 m^2/g of BET surface area and 1.32 cc/g of total pore volume. The effect of the activation method on the surface chemistry of the activated carbons was also studied. To measure the adsorption performance, liquid phase phenol adsorption experiments were conducted. The highest Langmuir monolayer adsorption capacity of 3.22 mmol/g was achieved by a KOH-activated sample.

13/00779 On the use of ethanol for evaluating microporosity of activated carbons prepared from Polish lignite

Carrott, P. J. M. *et al. Fuel Processing Technology*, 2012, 103, 34–38.
Microporous activated carbons prepared by KOH chemical activation or steam activation from lignite were characterized by adsorption of N_2 at 77 K and CO_2 at 298 K. Subsequently, the adsorption of ethanol was carried out and complemented by adsorption of benzene and cyclohexane. The isotherm analysis included application of the α_s method using ethanol reference data obtained here by also studying non-porous carbon blacks. The work confirmed that ethanol is an experimentally convenient adsorptive to use and leads to results in overall agreement with those obtained using other probe molecules. Of particular interest was the observation that ethanol can gain access to the whole microporosity even in the case of samples containing constricted micropore entrances. It was also possible to show that certain furnace carbon blacks contain intrinsic microporosity which is more difficult to unambiguously detect by adsorption of N_2 at 77 K. On the other hand, the results also suggested that the exact shape of the ethanol adsorption isotherm on a non-porous surface is more sensitive to the nature of the surface than has previously been found with other adsorptives.

13/00780 Physical characterization of activated carbons with narrow microporosity by nitrogen (77.4 K), carbon dioxide (273 K) and argon (87.3 K) adsorption in combination with immersion calorimetry

Silvestre-Albero, J. *et al. Carbon*, 2012, 50, (9), 3128–3133.

In order to get more insight into the characterization of nanoporous carbons by gas adsorption, the use of different probe molecules has been compared. A series of activated carbons with ranging porosity (burn-off) have been prepared from olive stones using CO_2 as activating agent and characterized using nitrogen and argon adsorption at low temperature (77.4 K for N_2 and 87.3 K for Ar) together with CO_2 adsorption at 273 K and immersion calorimetry into liquids of different molecular dimensions. Experimental results show that argon adsorption in narrow carbon micropores takes place at a higher relative pressure compared to nitrogen due to a weaker effective adsorption potential (lower strength of dispersion forces), including the absence of specific interactions of argon with the adsorbent surface. The application of advanced theoretical approaches based on the density functional theory (NLDFT and QSDFT) provides an accurate description of the pore-size distribution (PSD). The PSD obtained from the argon adsorption data at 87.3 K is in good agreement with immersion calorimetry measurements. The results demonstrate that argon adsorption at 87.3 K in combination with the application of advanced DFT methods (e.g. QSDFT) allows for a reliable characterization of the narrow microporosity in highly heterogeneous activated carbons.

13/00781 Post-treated incinerator bottom ash as alternative raw material for ceramic manufacturing

Schabbach, L. M. *et al. Journal of the European Ceramic Society*, 2012, 32, (11), 2843–2852.

New ceramics based on 60 wt% of alternative raw material derived from post-treated municipal solid waste incinerator bottom ashes and 40 wt% of refractory clay were studied. The chemical analysis of the compositions was evaluated by ICP. The thermal and densification behaviour of the ceramic batches were evaluated by DTA-TG and dilatometry techniques, respectively. After that, the degree of sintering at different temperatures and soaking times was evaluated in detail, measuring open and closed porosities, linear shrinkage and water absorption. The crystallinity at different temperatures (during heating and after cooling) and microstructure of the obtained samples were evaluated by high-temperature X-ray diffraction and scanning electron microscopy, respectively. For these new ceramics, the experimental results highlighted sintering range between 1190–1240 °C. In addition, the specimens demonstrated low water absorption and high crystallinity (with anorthite as main crystalline phase), leading to mechanical characteristics comparable to those of commercial ceramic products (bending strength > 40 MPa).

13/00782 Simulation and optimization of tyre-based steam activated carbons production for gas-phase polycyclic aromatic hydrocarbons abatement

Aranda, A. *et al. Chemical Engineering Journal*, 2012, 187, 123–132.

In this work, technical solutions for two remarkable environmental problems are undertaken: waste tyres (WT) valorization by producing steam activated carbons (AC), and gas-phase polycyclic aromatic hydrocarbons (PAH) abatement, by adsorption on those solids. First, the AC production process in a fixed bed reactor was modelled. For this purpose, the random pore model (RPM) was successfully applied, to model the solid evolution throughout the steam activation of WT. The model showed the capability of predicting with a high degree of accuracy both the conversion and the solid properties evolution, depending on the operational variables (i.e. temperature, steam concentration and time). The experimental results obtained in a lab-scale activation system allowed the model validation. Afterwards, the performance of the AC on the cyclic adsorption of naphthalene on gas phase was evaluated and related to the physical properties of the AC. These experiments confirmed the optima AC characteristics for naphthalene abatement. Since the physical properties of the AC can be accurately predicted with the proposed model, the activation process was optimized to enhance the final PAH adsorption capacity of the sorbents. Therefore, in this work, a useful tool for simulation and optimization of the AC production process for the specific application of PAH abatement has been developed.

13/00783 Strain dependent energy dissipation in multi-scale carbon fiber composites containing carbon nanofibers

Jang, J. S. *et al. Carbon*, 2012, 50, (11), 4277–4283.

This study investigates strain-dependent energy dissipation characteristics in carbon nanofibre (CNF) reinforced carbon fibre epoxy composites (multi-scale composites) by characterizing their viscoelastic properties and vibrational damping response. The air damping effect on the energy dissipation characteristics is also examined. The viscoelastic properties of epoxy containing two weight fractions (3 and 5 wt%) of added CNFs were characterized using dynamic mechanical analysis. Carbon fibre layers were then infiltrated with the two epoxy resins containing the CNFs to form multi-scale composites. A strain dependent loss factor behaviour of the multi-scale composites was observed in the dynamic cyclic testing due to CNF's stick–slip friction, showing a 53% increase in loss factor for the composites containing 5 wt% CNFs. The beam vibration test results also indicated an improvement in loss factor for the multi-scale composite beams relative to those without the CNF addition in the first two resonant frequencies. The multi-scale composite beams exhibit an increase in loss factor, up to 43%, at high amplitude excitation, while a reduction in loss factor was seen at low amplitude. These observed strain-dependent damping characteristics seem to result from both the stick–slip friction and the air damping effect.

13/00784 The adsorption characteristics of uranium hexafluoride onto activated carbon in vacuum conditions

Afsari, M. *et al. Annals of Nuclear Energy*, 2012, 46, 144–151.

The adsorption characteristics of uranium hexafluoride (UF_6) on activated carbon have been investigated under vacuum conditions for absolute pressure range of 10–35 mbar. The experiments were carried out for three different types of activated carbon. Evaluation of the experimental data in terms of adsorption kinetic showed that UF_6 gas adsorption by three types of activated carbon followed the pseudo-second-order-rate equation very well. The experimental isotherm data were analysed using the Langmuir, Freundlich and Henry equations. The results showed that the Langmuir isotherm model fitted the equilibrium data better than the other ones. At a temperature of 20 °C, the maximum adsorption capacity of the first, second and third activated carbon were 3387, 2198 and 2771 (mg/g), respectively. Adsorption studies were conducted at different temperatures to obtain the thermodynamic parameters. The results depicted the exothermic nature of adsorption and the process was feasible and spontaneous.

13/00785 The contribution of fly ash toward indoor radon pollution from concrete

Taylor-Lange, S. C. *et al. Building and Environment*, 2012, 56, 276–282.

Owing to concerns about radon exposure, there is a need for understanding risk associated with fly ash in concrete. Monte Carlo simulations were applied, based on the radium specific activity of concrete constituents taken from the literature, to predict probabilities for the radium specific activity and radon exhalation rate. The model was then used to predict the indoor radon concentrations and effective annual doses from two different slab-on-grade concrete floors, one with and one without fly ash, in a typical single-family home in the USA. Due to uncertainty in the literature-reported values, a sensitivity analysis was conducted varying the emanation fraction of the fly ash concrete floors. The results show that concrete floors made without fly ash and a 5% emanation fraction, resulted in 90% of the simulated homes having an indoor radon concentration of less than or equal to $2.3\,\mathrm{Bq\,m^{-3}}$ and an associated annual dose of less than or equal to $54\,\mu\mathrm{Sv\,y^{-1}}$. This annual dose represents 4% of the total annual background inhalation dose. A 25 wt% fly ash concrete with an emanation fraction of 3% achieved the same exposure probability, but higher assumed emanation fractions raised the exposure probability. In general, the predicted radon exposure from fly ash concrete suggests minimal population health effects. But, given the serious health effects of radon exposure the influence of fly ash on the emanation fraction and radioactive pollution indoors deserves further exploration.

13/00786 The influence of silver on the physicochemical and catalytic properties of activated carbons

Goscianska, J. *et al. Chemical Engineering Journal*, 2012, 189–190, 422–430.

Activated carbons prepared from walnut shells and coals have been used as supports for silver. The effects of precursor type, heating mode and activation temperature on the surface properties of the supports have been tested. Low-temperature nitrogen sorption, X-ray diffraction, scanning and transmission electron microscopy have been used to characterize a series of silver-modified samples. The results show that silver nanoparticles strongly determine textural properties as well as the amount and type of surface oxygen groups generated on the surface of the activated carbons. The impregnation of these activated carbons with silver species leads to the formation of attractive catalysts for the oxidation of cyclohexene with hydrogen peroxide.

13/00787 Wood ash as a magnesium source for phosphorus recovery from source-separated urine

Sakthivel, S. R. *et al. Science of the Total Environment*, 2012, 419, 68–75.

Struvite precipitation is a simple technology for phosphorus recovery from source-separated urine. However, production costs can be high if expensive magnesium salts are used as precipitants. Therefore, waste products can be interesting alternatives to industrially-produced magnesium salts. The authors investigated the technical and financial feasibility of wood ash as a magnesium source in India. In batch experiments with source-separated urine, 99% of the phosphate could be precipitated with a magnesium dosage of 2.7 mol Mg mol P^{-1}. The availability of the magnesium from the wood ash used in the experiment was only about 50% but this could be increased by burning the wood at temperatures well above 600 °C. Depending on the wood ash used, the precipitate can contain high concentrations of heavy metals. This could be problematic if the precipitate were used as fertilizer depending on the applicable fertilizer regulations. The financial study revealed that wood ash is considerably cheaper than industrially-produced magnesium sources and even cheaper than bittern. However, the solid precipitated with wood ash is not pure struvite. Due to the high calcite and the low phosphorus content (3%), the precipitate would be better used as a phosphorus-enhanced conditioner for acidic soils. The estimated fertilizer value of the precipitate was actually slightly lower than wood ash, because 60% of the potassium dissolved into solution during precipitation and was not present in the final product. From a financial point of view and due to the high heavy metal content, wood ash is not a very suitable precipitant for struvite production. Phosphate precipitation from urine with wood ash can be useful if (1) a strong need for a soil conditioner that also contains phosphate exists, (2) potassium is abundant in the soil and (3) no other cheap precipitant, such as bittern or magnesium oxide, is available.

05 NUCLEAR FUELS

Scientific, technical

13/00788 Application of the fractional neutron point kinetic equation: start-up of a nuclear reactor

Polo-Labarrios, M.-A. and Espinosa-Paredes, G. *Annals of Nuclear Energy*, 2012, 46, 37–42.

This study presents the behaviour of the variation of neutron density when the nuclear reactor power is increased using the fractional neutron point kinetic (FNPK) equation with a single-group of delayed neutron precursor. It is considered that there is a relaxation time associated with a rapid variation in the neutron flux and its physical interpretation of the fractional order is related with non-Fickian effects from the neutron diffusion equation point of view. The authors analysed the case of increase the nuclear reactor power when reactor is cold start-up which is a process of inserting reactivity by lifting control rods discontinuously. The results show that for short time scales of the start-up the neutronic density behaviour with FNPK shows sub-diffusive effects whose absorption are government by control rods velocity. For large times scale, the results shows that the classical equation of the neutron point kinetics over predicted the neutron density regarding to FNPK.

13/00789 Appropriate thermodynamic cycles to be used in future pressure-channel supercritical water-cooled nuclear power plants

Lizon-A-Lugrin, L. *et al. Nuclear Engineering and Design*, 2012, 246, 2–11.

As member of the Generation IV International Forum (GIF), Canada has decided to orient its efforts towards the design of a CANDU-type supercritical water-cooled nuclear reactor (SCWR). Such a system must run at a coolant outlet temperature of about 625 °C and at a pressure of 25 MPa. Even though several steam-cycle arrangements used in existing thermal-power plants have been discussed by many authors, none of the proposed cycles have been optimized and adapted to the pressure-channel SCWR concept. The present work is intended to fulfil this gap by including at least two alternative solutions of SCWR power cycles that could reheat the supercritical water in the reactor core to achieve a net mechanical power of 1200-MW. Thus, thermodynamic models for preselected power cycles, their validation among existing data as well as their optimization using an ‘evolutionary optimization’ technique based on genetic algorithms are presented and discussed.

13/00790 Assessment of the traditional neutron-diffusion core-analysis method for the analysis of the super critical water reactor

Shen, W. *Annals of Nuclear Energy*, 2012, 45, 1–7.

The key design quantities of the pressure-tube-based (PT-based) supercritical water reactor (SCWR) core design are expected to be computed with the traditional core-analysis code which solves the two-group neutron-diffusion equation by using lattice-homogenized cross sections calculated with the lattice code. Two issues may affect the accuracy of these computed quantities for the SCWR core: one is the two-energy-group neutron-diffusion theory; the other is the generation of lattice-homogenized properties with the lattice code based on the single-lattice-cell model without considering the effects of the environment. It has been illustrated that the single-lattice-cell method is not sufficiently accurate for heterogeneous core configurations when adjacent channels experience significant spectrum interaction. To ensure the qualification of these computed quantities for the SCWR core, a two-dimensional SCWR benchmark problem was set up (with the reference solution provided by the continuous energy Monte-Carlo code SERPENT) to assess the traditional neutron-diffusion core-analysis method. The assessment shows that the traditional two-group neutron-diffusion theory with the single-lattice-cell-based lattice properties is not sufficient to capture either the spectral change or the environment effect for the SCWR core. The solution of the eight-group neutron-diffusion equation by using lattice-homogenized cross sections calculated with the multicell model is considered appropriate for the analysis of the PT-based SCWR core.

13/00791 Beta decay of the fission product ^{125}Sb and a new complete evaluation of absolute gamma ray transition intensities

Rajput, M. J. *et al. Radiation Physics and Chemistry*, 2012, 81, (4), 370–378.

The radionuclide ^{125}Sb is a long-lived fission product, which decays to ^{125}Te by negative beta emission with a half-life of 1008 day. The beta decay is followed by the emission of several gamma radiations, ranging from low to medium energy, that can suitably be used for high-resolution detector calibrations, decay heat calculations and in many other applications. In this work, the beta decay of ^{125}Sb has been studied in detail. The complete published experimental data of relative gamma ray intensities in the beta decay of the radionuclide ^{125}Sb has been compiled. The consistency analysis was performed and discrepancies found at several gamma ray energies. Evaluation of the discrepant data was carried out using normalized residual and RAJEVAL methods. The decay scheme balance was carried out using beta branching ratios, internal conversion coefficients, populating and depopulating gamma transitions to ^{125}Te levels. The work has resulted in the consistent conversion factor equal to 29.59(13)%, and determined a new evaluated set of the absolute gamma ray emission probabilities. The work has also shown 22.99% of the delayed intensity fraction as outgoing from the 58 d isomeric 144 keV energy level and 77.01% of the prompt intensity fraction reaching to the ground state from the other excited states. The results are discussed and compared with previous evaluations. The present work includes additional experimental data sets that were not included in the previous evaluations. A new set of recommended relative and absolute gamma ray emission probabilities is presented.

13/00792 Building a dynamic code to simulate new reactor concepts

Catsaros, N. *et al. Nuclear Engineering and Design*, 2012, 246, 41–48.

Innovative nuclear reactor designs have been proposed, such as the accelerator driven systems (ADSs), the ‘candle’ reactors, etc. These reactor designs introduce computational nuclear technology problems the solution of which necessitates a new, global and dynamic computational approach of the system. A continuous feedback procedure must be established between the main inter-related parameters of the system such as the chemical, physical and isotopic composition of the core, the neutron flux distribution and the temperature field. Furthermore, as far as ADSs are concerned, the ability of the computational tool to simulate the nuclear cascade created from the interaction of accelerated protons with the spallation target as well as the produced neutrons, is also required. The new Monte Carlo code ANET (advanced neutronics with evolution and thermal hydraulic feedback) is being developed based on the GEANT3 high energy physics code, aiming to progressively satisfy all the above requirements. A description of the capabilities and methodologies implemented in the present version of ANET is given here, together with some illustrative applications of the code.

13/00793 CFD evaluation of turbulence models for flow simulation of the fuel rod bundle with a spacer assembly

Liu, C. C. *et al. Applied Thermal Engineering*, 2012, 40, 389–396.

Computational fluid dynamics (CFD) is increasingly being used in nuclear reactor safety (NRS) analyses to describe safety-relevant phenomena occurring in the reactor coolant system in greater detail. This paper presents the results of numerical issues such as mesh refinement, wall treatment and appropriate definition of boundary conditions, which exert great influence on the results of a CFD simulation. A high quality computational mesh was used to investigate the choice of turbulence model appropriate for the complex swirling flow in the rod bundle subchannels. The performance of various turbulence models are evaluated by calculation of the Nusselt number distribution in a fuel bundle. Comparison between numerical and experimental results of lateral and axial distributions for the Nusselt number obtained via turbulence model without near-wall functions is not sufficiently good, while agreement is found between the computational simulation of the realizable k–ε model with near-wall functions and the experimental measurements, for locations close to the support grid. As a result of this study, the most appropriate turbulence models and the best enhanced wall treatment for modelling reactor coolant systems can be determined.

13/00794 Damage parameters of structural materials in fusion environment compared to fission reactor irradiation

Sawan, M. E. *Fusion Engineering and Design*, 2012, 87, (5–6), 551–555.
Calculations were performed to quantify the damage parameters in the leading candidate structural and plasma facing materials when used in magnetic and inertial confinement fusion systems and when irradiated in fission reactors. The structural materials considered are ferritic steel, austenitic steel, vanadium alloy and SiC/SiC composite. Plasma facing materials included beryllium, tungsten, and carbon fibre composites. Atomic displacement damage and gas production rates are greatly influenced by the neutron energy spectrum. For the same neutron wall loading, atomic displacement damage is slightly lower in inertial fusion systems than in magnetic fusion systems but gas production is about a factor of two lower. In addition, much lower gas production is obtained in samples irradiated in fission reactors. The results help guide irradiation experiments in fission reactors to properly simulate the damage environment in fusion systems and facilitate extrapolating to the expected material performance in fusion systems.

13/00795 Evaluation of proliferation resistance of plutonium based on spontaneous fission neutron emission rate

Kimura, Y. *et al. Annals of Nuclear Energy*, 2012, 46, 152–159.
The proliferation resistance of plutonium can be enhanced by isotopic denaturing and one of the features of Pu isotopic denaturing is increasing of the spontaneous fission neutron emission rate. A high spontaneous fission neutron emission rate causes ‘predetonation’ in a nuclear explosive device, and it makes the designing and building of a nuclear explosive device more complicated. In this paper, the enhancement of Pu proliferation resistance by isotopic denaturing was evaluated based on spontaneous fission neutron emission rate using a simple nuclear explosive device model. The feature of spontaneous fission neutron was evaluated with probabilistic approach, and a new Pu categorization which makes enable to categorize plutonium by its isotopic compositions was proposed based on the evaluation results. The Pu categorization was applied to an evaluation of the proliferation resistance of plutonium produced in LWRs and FBRs using the evaluation function, ‘attractiveness’ for two types of plutonium; plutonium produced in typical LWRs and FBRs, and denatured plutonium produced by transmutation of minor actinides.

13/00796 Fusion yield measurements on JET and their calibration

Syme, D. B. *et al. Nuclear Engineering and Design*, 2012, 246, 185–190.
The power output of fusion experiments and fusion reactor-like devices is measured in terms of the neutron emission rates which relate directly to the fusion yield rate. Determination of such parameters requires a set of absolutely calibrated neutron detectors. At JET, the fission chamber neutron detectors were originally calibrated some 20 years ago by performing a set of *in situ* calibrations using neutron sources and the absolute calibration has been maintained since then by cross calibrations against activation system measurements. After this elapsed time and a succession of changes to the internal and external JET structures, the JET neutron yield calibration needs re-measurement. The purpose of this paper is to give an overview of the arrangements being developed to allow a new calibration to be made. A new, more detailed, calibration is being provided by means of an engineering programme of development of the robotic tools which will allow safe and accurate deployment of a strong ^{252}Cf source for the measurements. It is led by a scientific programme that seeks to better understand the limitations of the calibration, to optimize the measurements and other provisions, to provide corrections for perturbing factors and to ensure personnel safety and safe working conditions. Much of this work is based on an extensive programme of Monte Carlo calculations. These include the updating of previous JET models to provide continuity of comparison with previous understanding, the provision of fast models for side effect estimation and the development of a new more detailed JET model which will allow comparisons with the older more homogeneous model while coping with the demands of the new calibration.

13/00797 Grain boundary percolation modeling of fission gas release in oxide fuels

Millett, P. C. *et al. Journal of Nuclear Materials*, 2012, 424, (1–3), 176–182.
This paper presents a new approach to fission gas release modelling in oxide fuels based on grain boundary network percolation. The method accounts for variability in the bubble growth and coalescence rates on individual grain boundaries, and the resulting effect on macroscopic fission gas release. Two-dimensional representations of fuel pellet microstructures are considered, and the resulting gas release rates are compared with traditional two-stage Booth models, which do not account for long-range percolation on grain boundary networks. The results show that accounting for the percolation of saturated grain boundaries can considerably reduce the predicted gas release rates, particularly when gas resolution is considered.

13/00798 Kinematic and dynamic analysis of a serial-link robot for inspection process in EAST vacuum vessel

Peng, X. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 905–909.
The present paper introduces a serial-link robot which is named flexible in-vessel inspection robot (FIVIR) and developed for Experimental Advanced Superconducting Tokamak (EAST). The task of the robot is to carry process tools, such as viewing camera and leakage detector, to inspect the components installed inside of EAST vacuum vessel. The FIVIR can help to understand the physical phenomena which could be happened in the vacuum vessel during plasma operation and could be one part of EAST remote handling system if needed. The FIVIR was designed with the consideration of having easy control and a good mechanics property which drives it resulted in function modular design. The workspace simulation and kinematic analysis are given in this paper. The dynamic behaviour of the FIVIR is studied by multi-body system simulation using ADAMS software. The study result shows the FIVIR has ascendant kinematic and dynamic performance and can fulfil the design requirement for inspection process in EAST vacuum vessel.

13/00799 Measurement of absolute neutron flux in LWSCR based on the nuclear track method

Sadeghzadeh, J. *et al. Annals of Nuclear Energy*, 2012, 45, 166–169.
In the present paper, a solid state nuclear track detector is applied to measure the absolute neutron flux in the light water sub-critical reactor (LWSCR) in the Nuclear Science and Technology Research Institute. Up to now, the spectral parameters of thermal neutrons have been measured with activation foils that are not always reliable in low flux systems. The method investigated here is the irradiation method. Experiments concerning fission track detecting were performed. The experiment including neutron flux calculation method has also been investigated using the Monte Carlo code MCNP. The analysis shows that the values of neutron flux obtained by experiment are in fairly good agreement with the results obtained by MCNP. Thus, this method may be able to predict the absolute value of neutron flux at LWSCR and other similar reactors.

13/00800 Mechanical test on the ITER TF jacket

Qin, J. *et al. Cryogenics*, 2012, 52, (7–9), 336–339.
This paper focuses on mechanical tests on the ITER TF jacket 316LN stainless-steel material. During manufacture the conductor will be compacted, spooled and aged at approximately 650 °C after cable insertion. Therefore, sample jackets were prepared under compaction, stretching and annealing in order to simulate the manufacturing process of TF coils. The mechanical properties of the given material were measured at 4.2 and 300 K. Young’s modulus, yield strength (0.2% offset) and elongation are reported. SEM images showed that the TF jacket had more pronounced ductile behaviour. The elongation at failure is more than 30% at cryogenic temperature, showing that the TF jacket has high mechanical performance. It is concluded that the results complies with ITER requirements.

13/00801 Methodology investigations on uncertainties propagation in nuclear data evaluation

Dossantos-Uzarralde, P. *et al. Nuclear Engineering and Design*, 2012, 246, 49–57.
This paper discusses distinct ways of calculating nuclear cross-section variance–covariance matrices issued from the spherical optical model such as the deterministic sensitivity method and Monte Carlo method. It also discusses the selection of uncertain parameters using both the local sensitivity and global sensitivity methods (based on spectral methods using a polynomial decomposition) to determine the importance of the input parameters with respect to the final uncertainty. Finally, the authors attempt to evaluate the differences between the uncertainties generated by methods like least squares method and Bayesian method, both necessitating the use of experimental data. Discussing the results of simulation for the cross-section calculations of the major neutron reactions on ^{89}Y, interest was particularly focused on the mathematical rigour and quality of the uncertainties that were obtained.

13/00802 Overview of R&D activities on tritium processing and handling technology in JAEA

Yamanishi, T. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 890–895.

In JAEA, the tritium processing and handling technologies have been studied at the Tritium Process Laboratory. The main R&D activities are: the tritium processing technology for the blanket recovery systems; the basic tritium behaviour in confinement materials; and detritiation and decontamination. The R&D activities on tritium processing and handling technologies for a demonstration reactor (DEMO) are also planned to be carried out in the broader approach (BA) program by JAEA with Japanese universities. The ceramic proton conductor has been studied as a possible tritium processing method for the blanket system. The BIXS method has also been studied as a monitoring of tritium in the blanket system. The hydrogen transfer behaviour from water to metal has been studied as a function of temperature. As for the behaviour of high concentration tritium water, it was observed that the formation of the oxidized layer was prevented by the presence of tritium in water (0.23 GBq/cc). A new hydrophobic catalyst has been developed for the conversion of tritium to water. The catalyst could convert tritium to water at room temperature. A new Nafion membrane has also been developed by gamma-ray irradiation to get the strong durability for tritium.

13/00803 Preliminary design of hybrid energy reactor and integral neutron experiments

Li, M. *et al. Fusion Engineering and Design*, 2012, 87, (7–8), 1420–1424.

This study proposes a preliminary design for a fusion–fission hybrid energy reactor (FFHER), based on current fusion science and technology (with some extrapolations forward from ITER) and well-developed fission technology. The authors list design rules and put forward a primary concept blanket, with uranium alloy as fuel and water as coolant. The uranium fuel can be natural uranium, LWR spent fuel, or depleted uranium. The FFHER design can increase the utilization rate of uranium in a comparatively simple way to sustain the development of nuclear energy. The interaction between the fusion neutron and the uranium fuel is studied with the aim of to achieving greater energy multiplication and tritium sustainability. Other concept hybrid reactor designs are also reviewed. The authors design integral neutron experiments in order to verify the credibility of their proposed physical design. The combination of this program of research with the related thermal hydraulic design, alloy fuel manufacture, and nuclear fuel cycle programs provides the science and technology foundation for the future development of the FFHER concept in China.

13/00804 Progress of fusion nuclear technologies in the broader approach framework

Nishitani, T. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 535–542.

In the broader approach framework, the International Fusion Materials Irradiation Facility/Engineering Validation and Engineering Design Activities (IFMIF/EVEDA) project, the International Fusion Energy Research Center (IFERC) project, and the Satellite Tokamak project are implemented. In the IFMIF/EVEDA project, engineering design of IFMIF and engineering R&D include the construction and tests of an IFMIF prototype accelerator system up with a 9 MeV and CW deuteron beam, a liquid lithium test loop with free surface flow, and full scale irradiation test module including temperature control instrumentation. The commissioning of the EVEDA lithium test loop was completed in March 2011, and a lithium flow of ~5 m/s was obtained. As a part of the IFERC project, R&Ds on reduced activation ferritic/martensitic steels as blanket structural material, SiC_f/SiC composites as a flow channel insert material and/or alternative structural material, advanced tritium breeders and neutron multipliers, and tritium technology are carried out. At the beginning of 2011, the integrated DEMO design team was established among the IFERC project team and EU/JA home teams, where the design criteria, other design basis are discussed as an initial work. A high performance supercomputer with the peak performance of 1.3 Pflops is under installation at the Rokkasho BA site.

13/00805 R&D progress of Korean HCSB TBM

Cho, S. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 386–391.

Several R&Ds are being performed for Korean helium cooled solid breeder (HCSB) test blanket module (TBM) in the field of hydrogen isotopes permeation characteristics measurement in the helium purge line, joining technologies of structural materials, breeder pebble materials development, and the measurement of pebble bed characteristics. Electron beam welding for reduced activated ferritic–martensitic (RAFM) steel is evaluated to find optimal welding conditions. Also, a hydrogen permeation measurement apparatus is newly installed for the evaluation of the permeation barrier characteristics of stainless steel and RAFM steels. Two fabrication methods of lithium orthosilicate pebbles are investigated using slurry droplet methods. As methods of silicon carbide coating on the graphite pebble, microwave coating and chemical vapour deposition coating are evaluated. Two apparatuses are established to assess the thermo-mechanical properties of graphite and breeder pebble beds. The current status of R&D activities on these areas is introduced and the main progresses are addressed in this paper.

13/00806 Research on the designed emergency passive residual heat removal system during the station blackout scenario for CPR1000

Wang, M. *et al. Annals of Nuclear Energy*, 2012, 45, 86–93.

The concept of passive safety is put forward to improve the safety and reliability of the nuclear power plant. The secondary emergency passive residual heat removal system (EPRHRS) is an innovative design for China Pressurized Reactor (CPR1000), which can remove the core residual heat effectively and improve the inherent safety by passive methods when the station blackout (SBO) occurs. In this work, the EPRHRS, which is connected to the steam generator (SG) and consists of a heat exchanger (HX), a water tank and corresponding pipes and valves, was designed for CPR1000. The primary loop and EPRHRS were modelled using RELAP5/MOD3.4 to investigate the residual heat removal capability of the EPRHRS and the transient characteristics of the primary loop system in the event of the SBO accident. In addition, sensitivity studies were also performed to investigate effects of the main parameters of the EPRHRS on the transient behaviour of the primary loop and the EPRHRS. The effect of isolation valve opening time on the primary loop and the EPRHRS was also studied in the paper. The results of the study indicate that the optimized HX area is $200\,m^2$ when the EPRHRS water tank height is 10 m and the optimized isolation valve opening time is 30 s. The EPRHRS can remove the core decay heat from the primary loop effectively through the stable natural circulation established in the primary loop and the EPRHRS loop based on the calculation results. Therefore, it illustrates that the EPRHRS designed in the paper is effective and meaningful to CPR1000.

13/00807 Separation and treatment of ion-exchange resins used in cleaning systems of a research nuclear reactor

Flores-Espinosa, R. M. *et al. Chemical Engineering Journal*, 2012, 188, 71–76.

This study is based on experimental data from the elution of $^{60}Co^{2+}$ ions with Na^+ ions in mixed-bed columns packed with resins used in the cleaning system of a research nuclear reactor. The operational parameters for conditioning the resins were obtained by washing, separating cationic resins from anionic resins, and eluting radioactive ions from the cationic resins with a solution of 2 N NaCl. The ion-exchange behaviour of $^{60}Co^{2+}$–Na^+ was analysed by measuring the variation of the activity or concentration of radioactive cobalt in a column as a function of the amount of saline solution required to desorb the radioactive cobalt from the column. The linear model was applied to obtain the constants that describe the ^{60}Co desorption process.

13/00808 Study on deterministic response time design for a class of nuclear instrumentation and control systems

Chen, C. K. *et al. Annals of Nuclear Energy*, 2012, 46, 56–62.

This study deals with the problems of deterministic response time design for computer-based systems in the nuclear industry. The concurrent operations of a system are explicitly characterized as a Petri net (PN) model from the sequence diagram. In order to obtain the deterministic behaviour, linear logic is proposed. It describes state changes of the PN model precisely with symbolic time representation. Furthermore, an efficient design procedure is presented to meet the timing requirements of the entire system. An illustrative example of the bistable processor logic is provided to demonstrate the results obtained in previous sections and to reveal the practicability of the proposed approach. In the future, there could be a technique that attempts to combine the diagnostic and redundancy attributes to provide a completed design scheme for nuclear instrumentation and control systems.

13/00809 Subset Simulation of a reliability model for radioactive waste repository performance assessment

Cadini, F. *et al. Reliability Engineering & System Safety*, 2012, 100, 75–83.

This study shows an original application of the subset simulation (SS) technique on a model for the performance assessment of a near surface radioactive waste repository. The logic of the protective barriers of the repository is represented by a reliability model. The SS approach is founded on the idea that a small failure probability can be expressed as a product of larger conditional probabilities of some intermediate events; with a proper choice of the conditional events, the conditional probabilities can be sufficiently large to allow accurate estimation with a small number of samples. In the application, the method allows improving the efficiency of the random sampling for estimating the repository containment failure probability. Moreover, the peculiar set-partitioning scheme of the SS method is exploited for performing the analysis of the sensitivity of the failure probability estimate to the uncertain model parameters.

13/00810 The optimal number of thermal diffusion columns for deuterium recovery from H–D gas mixture in the countercurrent-flow Frazier scheme with the total sum of column heights fixed

Yeh, H.-M. and Hsu, C. C. *Progress in Nuclear Energy*, 2012, 59, 1–5.
The effect of the column number on deuterium recovery from H–D gas mixture in the countercurrent-flow Frazier scheme of thermal diffusion columns with the total sum of column heights fixed, has been investigated. The equations for predicting the optimal number of columns and the corresponding maximum separation have been derived. Considerable improvement in deuterium recovery is obtainable if the multi-column device with the optimal number of columns is employed, instead of using the single-column device with the same total sum of column heights, especially for the cases of higher volume flow-rate operation and larger total sum of column heights. Furthermore, countercurrent-flow operation is much better than forward-flow operation.

13/00811 Treatment of ion exchange resins used in nuclear power plants by super- and sub-critical water oxidation – a road to commercial plant from bench-scale facility

Kim, K. *et al. Chemical Engineering Journal*, 2012, 189–190, 213–221.
A supercritical water oxidation (SCWO) process has been developed to effectively reduce the quantities of waste ion exchange resins from the pressurized water reactors (PWR) in Korea. First of all, waste ion exchange resins were separated into cationic and anionic resins by a specific gravity difference in the fluidized bed. The separated resins were wet pulverized in a ball mill for 24 h to make uniformly dispersed slurry in high concentration. The optimal decomposition conditions for waste cationic and anionic resins from thermal power plants were obtained in a bench-scale facility of reactor of 220 mL volume. Then scale-up experiments were performed in a pilot plant with a 24 L reactor. The optimal values of such parameters as process temperature, process pressure, residence time, amount of oxidant, and amount of additives (NaOH and CH_3NO_2) for decomposition were determined by the pilot plant. The optimal process condition on cationic ion exchange was found under the sub-critical condition. The process temperature for anionic ion exchange resins was lowered to 515 °C. By using nitromethane as a denitrification agent, total-nitrogen (T-N) in the treated water was lowered as well as almost no NO_x was emitted from the exhausted gases. Based on the production rate and the stored amount of waste resins in the nuclear power plant ‘A’, a commercial facility with process capacity of 150 kg/h was designed in detail. This paper presents the procedure to scale-up from a bench-scale facility to a commercial plant and major check points in each stage.

Economics, policy, supplies, forecasts

13/00812 Activation analyses updating the ITER radioactive waste assessment

Pampin, R. *et al. Fusion Engineering and Design*, 2012, 87, (7–8), 1230–1234.
A study is reported which computes the radiation transport and activation response throughout the ITER machine and updates the ITER radioactive waste assessment using modern three-dimensional models and up-to-date methods. The latest information on component design, maintenance, replacement schedules and materials is adopted. The radwaste classification is revised for all the major components of ITER, as well as several representative port plugs. Results include categorization snapshots at different decay times, time histories of radiological quantities throughout the machine, and guidelines on interim decay times for components. All plasma-facing materials except tungsten are found to classify as type B due to the transmutation of their main constituents. Major contributors to the IRAS index of all materials are reported. Elemental concentration limits for type A classification of first wall and divertor materials are obtained; for the steels, only a reduction in service lifetime can reduce the waste class. Comparison of total waste amounts with earlier assessments is limited by the fact that analyses of some components are still preliminary; the trend, however, indicates a potential reduction in the total amount of waste if component segregation is demonstrated.

13/00813 Advantages and difficulties with the application of methods of probabilistic safety assessment to the power systems reliability

Čepin, M. *Nuclear Engineering and Design*, 2012, 246, 136–140.
The probabilistic safety assessment is a standardized and widely accepted method for assessing and improving the reliability and safety of complex technologies, which is particularly true for the nuclear and the aerospace industry. The number of its applications to reliability of power systems is increasing. The objective of the paper is to collect and present the advantages and difficulties with the application of methods of probabilistic safety assessment to power systems reliability. The methods which apply the features of fault tree analysis to reliability analysis of power systems are presented and compared. The results are discussed and evaluated. The main advantages are connected with the facts that the methods are relative simple, the models are mostly available and that the data is intensively collected, evaluated and can serve as an excellent support for the quantitative part of the analyses. The difficulties are connected with different nature of components interaction within the power system compared to the safety systems in a nuclear power plant and with the large complexity of the power system, which distinguishes the term reliability into its static and dynamic parts known as adequacy and security. The results show large impact of common cause failures. The lack of data for the evaluations in the field of common cause failures of power systems increases significantly the uncertainty of the results. The uncertainty of the results may be reduced by improved data collection and analysis similarly as it is done in the nuclear safety.

13/00814 An endothermic chemical process facility coupled to a high temperature reactor. Part I: proposed accident scenarios within the chemical plant

Brown, N. R. *et al. Nuclear Engineering and Design*, 2012, 246, 256–265.
Hydrogen generation using a high temperature nuclear reactor as a thermal driving vector is a promising future option for energy carrier production. In this scheme, the heat from the nuclear reactor drives an endothermic water-splitting plant, via coupling, through an intermediate heat exchanger. Quantitative study of the possible operational or accident events within the coupled plant is largely absent from the literature. In this paper, seven unique case studies are proposed based on a thorough review of possible events. The case studies are: (1) feed flow failure from one section of the chemical plant to another with an accompanying parametric study of the temperature in an individual reaction chamber, (2) product flow failure (recycle) within the chemical plant, (3) rupture or explosion within the chemical plant, (4) nuclear reactor helium inlet overcooling due to a process holding tank failure, (5) helium inlet overcooling as an anticipated transient without emergency nuclear reactor shutdown, (6) total failure of the chemical plant, (7) control rod insertion in the nuclear reactor. The qualitative parameters of each case study are outlined as well as the basis in literature. A previously published modelling scheme is described and adapted for application as a simulation platform for these transient events. The results of the quantitative case studies are described within part II of this paper.

13/00815 An overview of TACIS and PHARE nuclear safety projects related to thermalhydraulics

Pla, P. *et al. Progress in Nuclear Energy*, 2012, 58, 76–88.
Since 1991, the EC has been supporting the transition in eastern European and ex-Soviet countries to market economy through the Technical Assistance to the Commonwealth of Independent States (TACIS) and Poland Hungary Aid for Reconstruction of the Economy (PHARE) Programmes. One of the priority areas for TACIS and PHARE funding was nuclear safety. In this area the countries mainly concerned were Russia, Ukraine, Armenia, and Kazakhstan for TACIS; Bulgaria, Czech Republic, Hungary, Slovak Republic, Lithuania, Romania and Slovenia for PHARE. The final programme year of TACIS and PHARE was 2006. The projects of the 2006 programmes have reached completion in recent years. The TACIS Nuclear Safety and PHARE instruments were replaced in 2007 by the Instrument for Nuclear Safety Co-operation (INSC) and by the Instrument for Pre-Accession Assistance (IPA), for the period 2007–2013. In these programmes, the Joint Research Centre (JRC) of the European Commission (EC) was providing Technical and Scientific Expertise in the areas of Design Safety, On-Site Assistance, Assistance to the Nuclear Safety Authorities, Waste, Safeguards and Dissemination of project results for the EC Directorate General External Relations (DG RELEX), responsible for the TACIS strategy and multi-annual indicative programming, EC Directorate General EuropeAid Co-operation Office (DG AIDCO), in charge of annual programming and implementation of all TACIS projects and EC Directorate General Enlargement (DG ELARG), responsible for PHARE projects. Several TACIS and PHARE projects were focused on thermalhydraulic issues associated with VVER and RBMK reactor safety: accident analyses, severe accident analyses, accident management, experimental facilities and results databases, etc. These projects have included the application and evaluation of eastern codes in addition to the transfer, adaptation and use of western codes together with western technologies, analysis experience, know-how and training of eastern experts on the use of the codes, methodology and phenomena. This paper gives an overview of

some of the projects carried out so far during more than a decade of TACIS and PHARE assistance. It illustrates in particular the objectives and briefly the results obtained, assessing the areas covered, main achievements and summarizing the open issues.

13/00816 Cerium(III) molybdate nanoparticles: synthesis, characterization and radionuclides adsorption studies

Yousefi, T. *et al. Journal of Hazardous Materials*, 2012, 215–216, 266–271.

Cerium(III) molybdate nanostructure with average size about 40 nm was prepared by adding cerium(III) chloride and ammonium molybdate solutions under varying conditions. The product was characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infrared (FT-IR), thermogravimetric analysis (TGA) and Brunauere Emmette Teller (BET) techniques. Ion exchange capacity of the sample for potassium ion and distribution coefficients (K_d) for 23 metal ions were determined, the K_d values for Tl(I), Pb(II), Th(IV), U(VI) and Cs(I) ions were found to be sufficiently high for their removal from various effluents. The adsorption behaviour of the sample towards $Cs(I)_{134}$ species were studied. Finally, the binary separation of Dy(III)–U(VI), Sm(III)–Th(IV) and Cs(I)–Rb(I) and removal of $Cs(I)_{134}$ from the real sample were successfully achieved.

13/00817 Cost benefit analysis of advanced nuclear fuel cycle using linear programming optimization

Lee, J. *et al. Annals of Nuclear Energy*, 2012, 46, 116–120.

The advanced fuel cycle in nuclear energy means to reuse the spent nuclear fuel (SNF) from light water reactors (LWRs) as a fuel of fast reactors, such as sodium-cooled fast reactors (SFR). The advanced fuel cycle includes SFR and pyro-processing technology and the main purpose is to reduce the SNF accumulation. The cost competitiveness can originate from the reduction of SNF disposal cost and the uranium utilization cost. In this study, three important factors (recycling cost, disposal cost, and uranium price) were analysed and their interdependency was also investigated. The comparison between direct disposal and recycling clearly showed that the reduction of SNF and less required uranium can compensate the high cost of SFR and pyro-processing facility. However the cost and benefit of each system can be seen as trivial depending on who is judging this and also other considerations that may exist beyond cost. For detailed analysis and further extension, more logical and precise cost data will be necessary to support the methodology of optimization.

13/00818 Criticality safety analysis for a core catcher designed in Korea

Kim, S. H. *et al. Progress in Nuclear Energy*, 2012, 59, 66–74.

Corium is a molten mixture of portions of a reactor core generated by a core melting accident. Corium includes fissionable materials; therefore, a criticality safety analysis must be performed for the core catcher design. This study analyses the criticality safety of corium arranged in a core catcher developed in Korea. The corium composition was calculated for a 1400 MW_e nuclear power plant. There are several variables involved in the criticality evaluation of corium, thus conservative assumptions were used to reduce the number of variables. A criticality evaluation procedure was employed to assess the operational failure of the core catcher under different accident scenarios. Four kinds of scenarios were selected, and criticality evaluations were pursued for each case. The multiplication factors in each condition were calculated with MCNP5 code. Also, the code bias was calculated with the benchmark problems of 262 LEU experiments to account for the uncertainty of MCNP code. All evaluation results for the assumed scenarios showed that the core catcher satisfies the regulatory guidelines for criticality safety. The calculation results will be used in the design of a core catcher being developed in Korea. It is expected that the data calculated in this study can be used as reference data for criticality safety evaluations of core melting accidents. Also, the procedure for criticality safety evaluation proposed in this study can be utilized to establish regulatory guidelines in Korea.

13/00819 Experimental study on the hydro-mechanical behavior of Boom clay

Yu, H. D. *et al. International Journal of Rock Mechanics and Mining Sciences*, 2012, 53, 159–165.

In the context of research into deep nuclear waste disposal, Boom clay, a stiff soil from the Underground Research Laboratory in Mol, Belgium, has been studied in various works. In this paper, containing X-ray diffraction tests, oedometer tests, consolidated undrained shearing (CUS) tests and scanning electron microscopic (SEM) tests, a series of experimental studies intended to study the hydro-mechanical behaviour and micro fabric of Boom clay are presented. X-ray diffraction tests and SEM tests further highlight the high content of clay mineral of Boom clay (about 60% in average). Preconsolidation pressure, which is about 5.0 MPa, was determined by oedometer tests. High swelling property under hydro-mechanical coupling effect has been investigated on the clay samples during the CUS test, and also high viscous potential has been represented under shearing rate of 20 μm/min. SEM tests show that the microstructure of Boom clay arranged more directional and denser, and it can be observed clearly through the microstructure variation of pores and fissures.

13/00820 ITER safety and licensing update

Taylor, N. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 476–481.

Safety files were submitted by the ITER organization to the French nuclear safety authorities in March 2010 as a part of the licensing process. These included the preliminary safety report which presents the extensive safety analyses performed for ITER. The report has been the subject of examination by the authorities and their advisors, and discussions with them have been held on many topics. In the light of this process, this paper discusses some of the topics that remain prominent in the safety analysis of ITER. In particular, the provision of the two safety functions, confinement of radioactive material and limitation of exposure to radiation, is explained and some of the potential challenges to them are identified. Amongst these are the risks of fire and explosion, and external events such as earthquake and loss of all electric power. Provisions in the ITER design, together with the characteristics of fusion, ensure that a very good safety performance will be achieved.

13/00821 Life time estimation of SSCs for decommissioning safety of nuclear facilities

Jeong, K. S. *et al. Annals of Nuclear Energy*, 2012, 46, 244–247.

This paper suggests the estimation algorithm for the life time of structure, system and components (SSCs) for decommissioning safety of nuclear facilities using the performance data of linguistic languages and fuzzy theory. The fuzzy estimation algorithm of life time can be easily applicable but the estimated results depend on the relevant membership functions and performance characteristic functions. This method will be expected to be very useful for maintenance and decommissioning of nuclear facilities' SSCs as a safety assessment tool.

13/00822 Method for assessment of ageing based on PSA results

Volkanovski, A. *et al. Nuclear Engineering and Design*, 2012, 246, 141–146.

Method for prioritization of the nuclear power plant components considering the core damage frequency increase resulting from their ageing is developed and presented. The prioritization of the components is done with sensitivity coefficients obtained from their Fussel–Vesely importance measures and utilization of the Taylor expansion approach. Components are sorted depending on their contribution to the change of the core damage frequency of the plant. The overall change of the core damage frequency resulting from components ageing is assessed for different surveillance and replacement intervals. Developed method is applied on the reference probabilistic safety assessment model of the nuclear power plant. Components ageing rates from the TIRGALEX database are used as input data for the analysis. The main contributors to the increase of the core damage frequency are identified in the obtained results. The implications of extension of test intervals is assessed and presented. The limitations of the developed method and possibilities for future improvement are presented. The major issues considering the introduction of the ageing in the probabilistic safety assessment are discussed.

13/00823 Overview of the specialist assessments undertaken to support the JET safety case review

Vallory, J. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 407–411.

The Joint European Torus (JET) operates using deuterium as a fuel but has also operated in D–T mode where the fusion reaction is fuelled by deuterium and tritium. To justify the safety of the experiments, safety reports are produced and approved. The safety case has recently undergone a periodic safety review and preparations are being made to undertake a tritium campaign in 2015. To provide information regarding the compatibility between reactor-grade plasma and the materials facing the plasma, an 'ITER-like wall' was installed in JET comprising beryllium first wall tiles, solid tungsten and CFC tungsten coated tiles in the divertor region. The human factor analysis of key safety management requirements and fitness for purpose review of key safety related equipment is an ongoing work which is currently in progress to include the management requirements and equipment defined for the next D–T campaign. This paper presented an overview of the methodology and main conclusions/recommendations from these analyses. The importance of tritium awareness through review of procedures and training and the emphasis of preventative maintenance has been highlighted for the next D–T campaign. The first results of the loss of coolant accident analysis for in vessel cooling circuit breach with the 'state of the art' CATHARE code were presented. Parametric analysis on the physical and modelling parameters have to be conducted to draw final recommendations. The time evolution of the pressure in the vacuum vessel will be used as an input to the calculations of the beryllium–steam reactions to evaluate the impact of the beryllium wall on hydrogen deflagration.

13/00824 Preliminary results from a detritiation facility dedicated to soft housekeeping waste

Lefebvre, X. *et al. Fusion Engineering and Design*, 2012, 87, (7–8), 1040–1044.

Nuclear waste management has to be taken into account for fusion machine in tritium experimentations. Soft housekeeping waste is produced during both operating and dismantling phases and is contaminated by tritium under reduced (HT) and oxidized (HTO) forms. At CEA Cadarache, a lab-scaled facility has been built for soft housekeeping detritiation. The tritiated gas exhausted from the process described above is foreseen to be treated by a tubular Pd–Ag membrane reactor, for gaseous tritium recovery. Since this membrane reactor uses hydrogen as swamping gas the compatibility toward explosive hazard has to be taken into account. Then, this work presents a double objective. A first study is presented in order to identify the best conditions for the declassification of soft housekeeping waste, without tritium recovery. Experiments carried out at 120 °C are not efficient enough and do not allow one to choose the most efficient carrier gas. Some other tests are being currently performed at higher temperatures (150 °C). Moreover, due to safety issues, the use of air has to be avoided during membrane reactor implementation phase. Preliminary results obtained with hydrogen hazard-free carrier gases are also presented.

13/00825 Preliminary safety analysis of ex-vessel LOCA for the European HCPB TBM system

Jin, X. Z. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 454–460.

Ex-vessel loss of coolant accident caused by a double-ended pipe break of the helium coolant system inside port cell is considered as one of the most critical accident for the European Helium Cooled Pebble Beds Test Blanket Module (HCPB TBM) system. The resulting rapid helium blow-down causes an immediate block of the TBM cooling, which requires a prompt plasma shutdown. Even after the plasma shutdown the temperature can increase over the design limit and the accident sequence can lead up to a break of the TBM box protection after the failure of different protection systems. Thus air ingresses in the vacuum vessel from the damaged TBM system and steam from the surrounding ITER blanket and divertor structures. The evaluation of this sequence is very important for the definition of the correct protection strategy of the system. To consider all these different events a methodology has been developed in KIT combining different codes for a complete analysis of the accident. In particular, this paper shows an application of MELCOR code to model beryllium–steam reaction in a particular accidental sequence for the long term cooling.

13/00826 Safety approach in the EU test blanket systems design

Panayotov, D. *et al. Fusion Engineering and Design*, 2012, 87, (7–8), 1035–1039.

This paper considers the safety strategy and approach developed and followed in the design of the two European Union test blanket systems (TBS) designs describing its objectives, components and implementation. Addressing the safety in the early stage of the conceptual design of nuclear facilities is a well-recognized international practice and industrial project-level requirement for the successful completion of the licensing process within expected project cost and schedule. The impact of the early development of the safety approach, its implementation and monitoring in the design of nuclear device like the TBS is not limited to the safety assessment and licensing activities only. Safety approach plays indispensable role in reducing the overall project risk. It infiltrates the entire design process through the unavoidable interfaces between the design features and its safety level. In reality the entire process of the TBS development, design, technological demonstration and implementation is affected by the project team safety culture.

13/00827 Sensor development for position detection of diverse safety rod of fast reactor

Sharma, P. *et al. Annals of Nuclear Energy*, 2012, 46, 189–196.

The 500 MWe sodium-cooled prototype fast breeder reactor (PFBR) presently under advanced stage of construction has two diverse and independent shut-down systems. Each shutdown system comprises of independent sensing systems, control logic and drive mechanisms. The drive mechanism belonging to the first shutdown system is used for controlling reactor power and also for shutting down the reactor. It is known as control and safety drive rod mechanism (CSRDM). The mechanism belonging to the second shutdown system is used only for shutting down the reactor and is called diverse safety rod drive mechanism (DSRDM). The CSRDM has a potentiometer which is used to determine the position of the control and safety rod (CSR). The free fall time of control and safety rod can also be measured with the help of the potentiometer. Constraint of putting similar type of instrument in DSRDM has prohibited position detection of the diverse safety rod (DSR) as well as measurement of free fall time of the DSR. However, the centre has embarked on development of three different techniques to detect the position and free fall time of DSR. These techniques are Kalman filtering technique using neutronic signal to detect position of the DSR, measurement of acoustic signal which is produced when the DSR hits the dashpot and the eddy current based technique. Description of development of eddy current-based sensor to detect position and free fall time of the DSR is the main aim of this paper. The sensor consists of five coils which are inductively coupled. The change in position of the DSR causes a change in inductance of the coil and hence a voltage induced in the coil. The measurement of the coil voltage reveals the position of the DSR. Sodium testing of the sensor has been carried out on a 1:1 model of the sensor. The performance of the sensor at various temperatures and frequencies has been studied and found satisfactory. The sodium testing has shown encouraging results and has proven the feasibility of using such a sensor for the reactor application. The piston of the DSR is made of modified 9Cr–1Mo magnetic steel. A sensor winding is placed around the dashpot, the inductance of the winding changes when the DSR is deposited in the dashpot. Transformer coupling between two windings is then used to measure the inductance change of the sensor winding to facilitate non-contact measurement. The winding configuration has been chosen such that the signal can be picked-up even when there is misalignment between the coils due to thermal and radiation induced dimensional changes.

13/00828 Tc and Re behavior in borosilicate waste glass vapor hydration tests II

Buechele, A. C. *et al. Journal of Nuclear Materials*, 2012, 429, (1–3), 159–165.

Technetium (^{99}Tc) is a significant environmental risk factor to consider for nuclear waste disposal repositories. Rhenium (Re), in the same column of the periodic table as Tc, is often used as a non-radioactive surrogate for Tc. Six waste glasses containing both Tc and Re were synthesized under a variety of redox conditions to produce different distributions of Tc and Re oxidation states. These glasses were exposed to vapour hydration tests (VHT) at 200 °C for 23–30 days; and the Tc and Re oxidation state, coordination environment, and spatial distribution within the altered coupons were determined. Compared with the original glasses, the corresponding VHT samples showed substantial reduction of Tc species, except where the original glass contained only reduced Tc (Tc^{4+}). Similar to earlier findings, Tc is more sensitive to redox conditions than Re with respect to both glass synthesis conditions and VHT alteration processes. Glasses that originally contained more oxidized Tc (near 100% Tc^{7+}) showed the most Tc enrichment in the altered VHT sample layers, where Tc was largely reduced to Tc^{4+}. Re is generally more oxidized than Tc in the samples measured and has similar spatial distributions as Tc in some VHT samples, while having very different spatial distributions compared with Tc in others. Glasses that originally had a distribution of Tc oxidation states (approximately 1:1 Tc^{4+} to Tc^{7+}), had Tc concentrations in the VHT altered layers that were approximately equal to or less than those found in the unaltered glass. However, in the same samples, Re concentrations were highest in the altered layers. Overall, with regard to spatial distributions within the altered VHT layers, the behaviour of Re was not a good predictor of Tc behaviour. Therefore, at least under VHT conditions, using Re as a non-radioactive surrogate for Tc in borosilicate waste glasses can provide misleading results.

13/00829 The economic effects of the deferred disposal of spent fuel in Korea

Kim, S. K. *et al. Progress in Nuclear Energy*, 2012, 59, 12–18.

The present study analyses the economic effects concerning deferred disposal of spent fuel through long-term storage. According to the cost analysis, a scenario that a 90-year deferral of an HLW (high-level waste) repository construction in favour of a long-term storage of spent fuel would be economically preferable to another scenario based on the year 2040 chosen as the starting point for construction on a repository. That is, the former scenario would cost about half that of the latter. This finding is an estimated result from an economic perspective only, assuming the disposal of 20,000-ton PWR spent fuel and 16,000-ton CANDU spent fuel. Still, it seems necessary to elicit proper term of storage for radioactive waste in order to comply with the so-called polluter-pays principle that the current generation cannot pass on its radioactive waste to the next generation.

13/00830 Validation test case generation based on safety analysis ontology

Fan, C. F. and Wang, W. S. *Annals of Nuclear Energy*, 2012, 45, 46–58.

Validation tests in the current nuclear industry practice are typically performed in an *ad hoc* fashion. This study presents a systematic and objective method of generating validation test cases from a safety analysis report (SAR). A domain-specific ontology was designed and used to mark up a SAR; relevant information was then extracted from the marked-up document for use in automatically generating validation test cases that satisfy the proposed test coverage criteria; namely, single parameter coverage, use case coverage, abnormal condition coverage, and scenario coverage. The novelty of this technique is its systematic rather than *ad hoc* test case generation from a SAR to achieve high test coverage.

13/00831 VVER 1000 SBO calculations with pressuriser relief valve stuck open with ASTEC computer code

Atanasova, B. P. *et al. Annals of Nuclear Energy*, 2012, 46, 121–127.

Station Blackout calculations without the availability of hydro accumulators were investigated for a VVER-1000 (V320) reactor with the ASTEC V1.3R2 and ASTEC V2 computer code. ASTEC predictions have been studied for the in-vessel phase of the accident until vessel failure. The new version of ASTEC V2 predicts significantly earlier core degradation and vessel failure compared to the old ASTEC V1.3.2 for SBO scenario. There is significantly less hydrogen released by the new ASTEC V2 compared to the old ASTEC V1.3.2. It could be explained by using different oxidation correlations in both versions.

13/00832 Safety of fusion magnets: model experiments to high current arcs at ITER busbars and feeder lines

Klimenko, D. and Pasler, V. *Fusion Engineering and Design*, 2012, 87, (5–6), 675–679.

Electric arcs moving along the power cables (the so-called busbars) of the toroidal field (TF) coils of ITER may reach and penetrate the cryostat wall. Model experiments with the VACARC (VACuum ARC) device were initiated to investigate the propagation and destruction mechanisms of busbar arcs in small scale. These experiments are intended to support the development and validation of a numerical model. The present setup simulates the fact that the busbar is contained by an inner and an outer feeder tube which absorb radiated energy and will be in contact with hot metal melt from the busbar. The tubes may also direct the hot plasma jet flow of the arc as long as they are intact. Experiments at scaled values for tube diameter, wall thickness and expected power density suggest serious damage to the inner feeder tube by the arc. This asks for further investigations that include the outer tube, too. The extent of damage to the tube samples depends on arc power, as expected. At high currents an additional luminous effect takes place, which is attributed to a reaction of oxygen and hydrogen probably set free from the dissociation of the insulation resin by the heat of the arc.

06 ELECTRICAL POWER SUPPLY AND UTILIZATION

Scientific, technical

13/00833 A full-space conformal mapping for the calculation of series impedance of overhead transmission lines and underground cables

Bonyadi-ram, S. *et al. Electric Power Systems Research*, 2012, 91, 95–103.

This paper introduces a two-dimensional conformal transformation scheme for the parameter extraction of an arbitrary overhead transmission line or underground cable in an unbounded lossy space. The quasi-magnetic Helmholtz equation is solved using the finite element method (FEM). A modified bilinear transformation is employed to transform the unbounded domain to a bounded domain that is more efficiently handled in FEM simulations. Due to conformality of the transformation, the magnetic stored energy, which is used to calculate the per-unit-length inductance matrix is independent from the mapping factor while the longitudinal current and its corresponding dissipated energy, which is used to calculate the per-unit-length resistance matrix are functions of the mapping factor. Numerical results for an overhead transmission line and a buried multiconductor cable are compared with those calculated using Carson's approximation and Wedepohl's formula from near DC to the high-frequency range.

13/00834 A fuzzy logic energy management system for polygeneration microgrids

Kyriakarakos, G. *et al. Renewable Energy*, 2012, 41, 315–327.

This paper presents the design and testing through simulation of a fuzzy logic energy management system (FLEMS) for an autonomous polygeneration microgrid. In this microgrid the energy is produced by photovoltaics and a wind turbine and the rest of the components include a battery bank, a proton exchange membrane (PEM) fuel cell, a PEM electrolyser, a metal hydride tank and a reverse osmosis desalination unit using energy recovery. The microgrid covers the electricity, transport and water needs and thus its products are power, hydrogen as transportation fuel and potable water through desalination. Initially an ON/OFF approach to the management and control of the devices was adopted. In this paper a new approach based on fuzzy logic was designed and tested through simulation. The devices being managed are the fuel cell, desalination unit and electrolyser unit. A design tool based on TRNSYS 16, Matlab, GenOpt 2.0 and TRNOPT was developed using a particle swarm optimization (PSO) method. Two microgrids were sized using this tool in order to compare the performance of FLEMS with the ON/OFF approach. The results show that FLEMS utilizes the available energy in the system better and the components' sizes are, thus, considerably decreased.

13/00835 A heuristic method of variable selection based on principal component analysis and factor analysis for monitoring in a 300 kW MCFC power plant

Jeong, H. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11394–11400.

In a commercialized 300 kW molten carbonate fuel cell (MCFC) power plant, a univariate alarm system that has only upper and lower limits is usually employed to identify abnormal conditions in the system. Even though univariate alarms have already been adopted for system monitoring, this simple monitoring system is limited for using in an extended monitoring system for fault diagnosis. Therefore, based on principal component analysis (PCA), a recursive variable grouping method for a multivariate monitoring system in a commercialized MCFC power plant is presented in this paper. In terms of development, since a principal component analysis model that contains all system variables cannot isolate a system fault, heuristic recursive variable selection method using factor analysis is presented here. To verify the performance of the fault detection, real plant operations data are used. Furthermore, comparison between type 1 and 2 errors for four different variable groups demonstrates that the developed heuristic method works well when system faults occur. These monitoring techniques can reduce the number of false alarms occurring on site at MCFC power plant.

13/00836 An improved robust model for generator maintenance scheduling

Ekpenyong, U. E. *et al. Electric Power Systems Research*, 2012, 92, 29–36.

The maintenance schedule of generators in power plants needs to match the electricity demand and ensure the reliability of the power plants at a minimum cost of operation. In this article, a reliability criterion modified generator maintenance scheduling (MGMS) model is formulated with additions and modifications made to the classic generator maintenance scheduling (GMS) model. The MGMS model includes modified maintenance window constraints with some newly added constraints. A comparison is then made between the MGMS model and the classic GMS model when both models are applied to a 21-unit test system. The results show that the MGMS model gives more reliable solutions than the GMS model. Due to the reliable results of the reliability criterion MGMS model, a robust model using economic cost objective function is formulated. To illustrate the robustness of the formulated MGMS model, the maintenance of the Arnot Power Plant in South Africa is scheduled with open loop and closed loop controllers. Both controllers satisfy all the constraints but the closed loop results are better than the open loop results.

13/00837 Bioconversion of the cellulose containing waste into electricity through the intermediate hydrogen production

Voronin, O. G. *et al. International Journal of Hydrogen Energy*, 2012, 37, (14), 10585–10589.

The bioreactor cell combined a hydrogenase-based fuel electrodes and a microbial bioreactor was developed. It was shown that the enzyme electrodes are able to convert hydrogen produced by bacteria into electricity without any additional purification steps. Paper wastes were used as a carbon source. Maximum power output achieved was of 200 $\mu W/cm^2$. Fuel cell remains at least 70% of the initial power during 72 h. The level of generated power is significantly higher than the reported for microbial fuel cells. The results demonstrate the possibility to generate power at a high rate with a variety of organic compounds used.

13/00838 Carbon monoxide generation, dispersion and exposure from indoor operation of gasoline-powered electric generators under actual weather conditions

Wang, L. *et al. Building and Environment*, 2012, 56, 283–290.

Gasoline-powered electric generators are widely used during power outages such as those caused by hurricanes and winter storms. Based on currently available data, about 95% of generator-related carbon monoxide (CO) fatalities were associated with operating carburetted, spark-ignited and gasoline-powered generators in enclosed spaces. To investigate the indoor CO exposure associated with running a generator indoors, the generation of CO was measured from a generator in an enclosed shed. Correlations of CO generation and O_2 consumption rates were developed as functions of O_2 level and actual generator load output. An indoor air quality and ventilation model was then used to predict the air change rates and CO levels in the shed, which were then compared with measured values. This study also used the simulation model to calculate CO generation and dispersion, and occupant exposures to CO, with a generator running in the garage of a house during weather conditions consistent with the days after Hurricane Katrina in the summer of 2005. For the simulation conditions, it was found that the resultant CO could reach dangerous levels in most rooms of the house about 2 h after the generator started.

13/00839 Design of a robust and efficient power electronic interface for the grid integration of solar photovoltaic generation systems

Pacas, J. M. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10076–10082.

Nowadays, the penetration of photovoltaic (PV) solar power generation in distributed generation (DG) systems is growing rapidly. This condition imposes new requirements to the operation and management of the distribution grid, especially when high integration levels are achieved. Under this scenario, the power electronics technology plays a vital role in ensuring an effective grid integration of the PV system, since it is subject to requirements related not only to the variable source itself but also to its effects on the stability and operation of the electric grid. This paper proposes an enhanced interface for the grid connection of solar PV generation systems. The topology employed consists of a three-level cascaded Z-source inverter that allows the flexible, efficient and reliable generation of high quality electric power from the PV plant. A full detailed model is described and its control scheme is designed. The dynamic performance of the designed architecture is verified by computer simulations.

13/00840 Design of innovative power conditioning system for the grid integration of thermoelectric generators

Molina, M. G. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10057–10063.

A novel power conditioning system of a grid-connected thermoelectric generator (TEG) system to simultaneously and independently control the active and reactive power flow in the distribution grid has been studied and implemented. A real detailed model and a novel multilevel control scheme based on a full decoupled current control of the inverter in *d*–*q* coordinates with a maximum power point tracking control of the TEG array were proposed. Dynamic system simulation studies demonstrate the effectiveness of the proposed models and control algorithms. The fast response of the PCS and the enhanced performance of the described control techniques allow taking full advantage of the TEG system as a distributed generator. The presented single-stage power conditioning system topology with self-boost capabilities offers a simple and effective alternative over the conventional two-stage one for interfacing the TEG devices with the AC utility grid. The advantages of this topology include a better power conversion efficiency, higher reliability, inherent short circuit protection and a reduction of the volume and weight of the entire system.

13/00841 Dynamic simulation of MEA absorption process for CO_2 capture from power plants

Harun, N. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 295–309.

Carbon dioxide (CO_2) emissions reduction from combustion fossil fuel power plants is a key aspect in the stabilization of global climate change. Post-combustion CO_2 capture from fossil fuel power plants using amine-based solvents, typically monoethanolamine (MEA), is one of the most promising technologies for the abatement of CO_2 gas. In this work, a dynamic MEA absorption process model has been developed to predict the dynamic behaviour of the CO_2 capture process. The resulting dynamic model was used to study the transient response of the MEA absorption process to changes in the flue gas flow rate and the reboiler heat duty. The changes in flue gas flow rate and reboiler heat duty are key process variables that affect the lean loading, liquid to gas ratio and percentage of CO_2 removal. To represent the actual operation of a power plant, the dynamic response of the MEA absorption process to a sinusoidal change in the flue gas flow rate was also considered in the present analysis. The results show that the changes between the reboiler heat duty and CO_2 removal follows a ratio of approximately 1:1.4. Also, the lean loading stream entering the absorber unit is key to maintain the feasible operation of the system. Moreover, the energy performance of the process (Joules per mole of CO_2 captured) is directly affected by the operation of the reboiler. The outcomes from this study provide insights regarding the dynamic behaviour of this process and can be used as the basis to develop other aspects related to the dynamic operation of this plant, e.g. to develop control strategies for this system.

13/00842 Effects of draw solutions and membrane conditions on electricity generation and water flux in osmotic microbial fuel cells

Ge, Z. and He, Z. *Bioresource Technology*, 2012, 109, 70–76.

This study provided an early effort to investigate the draw solutions as catholytes, FO membrane conditions, and backwash for membrane cleaning in an osmotic microbial fuel cell (OsMFC). The results demonstrated that sodium chloride was a suitable candidate as a catholyte solute with good performance in both electricity generation and water flux, although its pH required buffering via acid addition. Adding a small amount of hydrochloric acid decreased the catholyte pH from 9.0 to 2.5 and increased the current generation by 50%, but did not affect water flux. It was also found that the fouled FO membrane improved electricity generation but lost the function of water flux. The damaged FO membrane resulted in a water flux of 0.39 LMH, much lower than 2–3 LMH with a new FO membrane. Backwash with adding NaCl (0.2–0.5 M) into the anolyte was examined but did not obviously alleviate membrane fouling.

13/00843 Electrical and thermal characterization of a novel high pressure gas cooled DC power cable

Rodrigo, H. *et al. Cryogenics*, 2012, 52, (4–6), 310–314.

High-temperature superconductors (HTS) allow power cables of substantially higher current density than conventional copper or aluminium cables. This is important for applications where a low mass and a low volume are critical such as naval, aeronautical and space applications. The novel type of cable under consideration is cooled by gaseous helium at elevated pressure. Helium is known for having poor electric breakdown strength; therefore the dielectric capabilities of this type of cable must be tested under conditions similar to the envisaged operation. In order to study the dielectric performance the authors have designed and built a novel high pressure cryostat rated at 2.17 MPa which has been used for testing model cables of lengths of up to 1 m. The cryostat is an open system where the gas is not recirculated. This allows maintaining a high purity of the gas. The target temperature range is between 40 and 70 K. This substantially increases the critical current density of the HTS compared to 77 K, which is the typical temperature of cables cooled by liquid nitrogen. The cryostat presented allows for adjusting the temperature and keeping it constant for the time necessary to run a complete dielectric characterization test. The authors give a detailed description of the cryostat. Measurements of partial discharge inception voltages as well as the temperature distribution along the model cables as a function of time are presented. Tests showed that the thermal insulation characteristics of this cryostat were sufficient for the dielectric tests of up to 1 h duration. The partial discharge inception voltage (PDIV) of the high-voltage bushing was about 16 kV. These values are well within the design requirements.

13/00844 Experimental study on effect of electric field on hydrate nucleation in supercooled tetra-n-butyl ammonium bromide aqueous solution

Kumano, H. *et al. International Journal of Refrigeration*, 2012, 35, (5), 1266–1274.

The effect of an electric field on hydrate nucleation in supercooled tetra-*n*-butyl ammonium bromide (TBAB) aqueous solution was investigated experimentally. Experiments were carried out by charging electrodes inserted into a test tube containing TBAB aqueous solution using a DC voltage. The electrode material (copper, aluminium, nickel, iron and gold), value of applied voltage and sample concentration were varied as the experimental parameter. When the sample was maintained under a supercooled state, the DC voltage was applied directly to the TBAB aqueous solution for 1 min. It was found that the probability of nucleation depends on the electrode material. The probability of nucleation is especially high in the case of the Cu electrode. It was also found that the probability of nucleation of type 2 TBAB hydrate is lower than that of type 1 hydrate under these experimental conditions.

13/00845 Identifying unstable region of operation in a micro-grid system

Acevedo, S. S. and Molinas, M. *Energy Procedia*, 2012, 20, 237–246.

This paper presents the stability analysis based on impedance representation of a single phase inverter operating as voltage source, where the Nyquist criteria can be applied. The method can be used to study the stability of a micro-grid dominated by power electronics in isolated operation mode. First, a small signal input impedance model is described. The second methodology applies no energy storage at the AC and DC side of the inverter. For two methods, a comparative evaluation with the measured impedance was realized. The obtained results show that the proposed method of no energy storage can be employed in the studies of stability for micro-grid systems.

13/00846 Integrating renewable energy technologies to support building trigeneration – a multi-criteria analysis

Chua, K. J. *et al. Renewable Energy*, 2012, 41, 358–367.

This paper evaluates the potential of hybridizing renewable technologies to support trigeneration. A model for trigeneration has been developed for simulation and evaluation. The developed trigeneration system aims to be self-sustaining where cooling, heating and power needs of a commercial building are simultaneously fulfiled. The system comprises four key sub-systems, namely, photovoltaic-thermal, solar-thermal, fuel cell, microturbine and absorption chiller-water system. Conventionally, a trigeneration system is analysed based on cost reduction without considering the energy used and the level of carbon dioxide emission. In contrast, this paper presents an analysis of the system using a multi-criteria analysis approach in terms of: (1) operation cost reduction, (2) energy saving; and (3) minimum environmental impact. For this trigeneration system layout, the result has indicated that a trigeneration system consisting of 80% of microturbine, 10% of photovoltaic-thermal and 10% fuel cell to be the optimum system composition in terms of reducing operational cost, improving energy saving and minimizing environment impact. The methodology portrayed in this study provides a pragmatic approach in the design of renewable energy systems to support trigeneration applications.

13/00847 Microbial carbon capture cell using cyanobacteria for simultaneous power generation, carbon dioxide sequestration and wastewater treatment

Pandit, S. *et al. Bioresource Technology*, 2012, 107, 97–102.

Microbial carbon capture cells (MCCs) were constructed with cyanobacteria growing in a photo biocathode in dual-chambered flat plate mediator-less MFCs separated by an anion exchange membrane from the anode compartment containing *Shewanella putrefaciens*. The performance of the MCC with *Anabaena* sparged with CO_2–air mixture was compared with that of a conventional cathode sparged with air only. The power densities achieved were $57.8\,mW/m^2$ for *Anabaena* sparged with a CO_2–air mixture, $39.2\,mW/m^2$ for CO_2–air mixture sparging only, $29.7\,mW/m^2$ for *Anabaena* sparged with air, and $19.6\,mW/m^2$ for air sparging only. The pH of the cathode containing *Anabaena* gradually increased from 7 to 9.12 and power generation decreased from 34.7 to $23.8\,mW/m^2$ 17 due to pH imbalance associated voltage losses without CO_2–air mixture sparging. Sparging with a 5% CO_2–air mixture produced maximum power of $100.1\,mW/m^2$. In addition, the power density of MCC increased by 31% when nitrate was added into the catholyte.

13/00848 Microbial desalination cells for improved performance in wastewater treatment, electricity production, and desalination

Luo, H. *et al. Bioresource Technology*, 2012, 105, 60–66.

The low conductivity and alkalinity in municipal wastewater significantly limit power production from microbial fuel cells (MFCs). This study integrated desalination with wastewater treatment and electricity production in a microbial desalination cell (MDC) by utilizing the mutual benefits among the above functions. When using wastewater as the sole substrate, the power output from the MDC ($8.01\,W/m^3$) was four times higher than a control MFC without desalination function. In addition, the MDC removed 66% of the salts and improved COD removal by 52% and Coulombic efficiency by 131%. Desalination in MDCs improved wastewater characteristics by increasing the conductivity by 2.5 times and stabilizing anolyte pH, which therefore reduced system resistance and maintained microbial activity. Microbial community analysis revealed a more diverse anode microbial structure in the MDC than in the MFC. The results demonstrated that MDC can serve as a viable option for integrated wastewater treatment, energy production, and desalination.

13/00849 Nanosecond reversible solid state switches capable of handling MJ of energy

Metz, R. *et al. Journal of the European Ceramic Society*, 2012, 32, (10), 2443–2450.

The theoretical applicability of the Schottky thermionic emission model to electronic transport at tin dioxide grain boundaries is addressed. Firstly, the theoretical behaviour of the barrier height $\Phi_{(v)}$ versus applied voltage is determined for a single grain boundary. Next the authors predict the current density–voltage characteristics as a function of temperature, demonstrating good correlation between experimental and theoretical results. The model carried out has the advantage that it contains no adjustable parameters. Agreement with experimental results from optimized polycrystalline ceramics gives strong evidence for the double-depletion-layer/thermionic-emission model. Moreover, this study emphasizes the importance of the direct large-bandgap of doped SnO_2 in surge-arrester applications, and gives credibility to the analogy between the apparent behaviour of doped SnO_2 and doped ZnO varistors. Doped polycrystalline tin oxide ceramic is the first material to compete with doped ZnO in the medium and high voltage applications for surge arresters.

13/00850 Optimizing the process for emptying carbon dioxide cylinders used for hydrogen sweeping in high-power electrical generators

Blanco, J. M. and Peña, F. *Applied Thermal Engineering*, 2012, 39, 132–139.

High-power alternators in large thermal power plants are generally cooled by hydrogen. Operating an electric power generator produces large amounts of heat that must be removed to improve efficiency. This means that the filling and emptying process needs to be performed in an inert atmosphere. Operating experience has shown that carbon dioxide is the most suitable fluid for this purpose because its molecular weight is considerably higher than that of hydrogen. On average, 90% of the contents of each cylinder are in a liquid state. As the process for discharging the cylinder proceeds, the gas progressively gets cool and may give rise to what is referred to as 'dry ice', rendering useless the rest of the content. This article describes the study and implementation of an experimental solution that optimizes the emptying of these cylinders in a power plant, thereby making a considerable saving because of their better exploitation.

13/00851 Over-current relay implementation assuring fast and secure operation in transient conditions

Lotfifard, S. *et al. Electric Power Systems Research*, 2012, 91, 1–8.

In order to reduce hazardous effects of over current caused by faults, faster operation of over-current protections is desirable which means maximum sensitivity of the over-current relays to the current and a minimum reaction time. This high sensitivity may lead to operation of relays in normal transient events, such as transformers energizing and induction motors starting. Therefore, proper methods must be used to prevent mal-trip of the relays, due to these transient currents. This paper presents a new method to discriminate over currents caused by fault from transformer energizing and induction motors starting. In this method, a criterion function is introduced in terms of variation of fundamental component amplitude of current signal over consecutive segments. The criterion function is then used in over-current protection, and faults are precisely discriminated from non-fault switching. The performance of this method is demonstrated by simulation of different faults and switching conditions on the IEEE 13 bus test system using electromagnetic transients program and field measured data.

13/00852 Short-term hydrothermal generation scheduling solved with a mixed-binary evolutionary particle swarm optimizer

Hinojosa, V. H. and Leyton, C. *Electric Power Systems Research*, 2012, 92, 162–170.

In this paper, a mixed-binary evolutionary particle swarm optimizer is applied to short-term hydrothermal generation scheduling problem (HGSP) in power systems. The HGSP has been formulated taking into account two decision variables simultaneously: water discharge (continuous) and thermal states (binary). The constraint handling technique used in the evolutionary algorithm is based on a strategy to generate and to keep the decision variables in feasible space through the correction operators, which were applied to hydro, thermal and system constraints. Such operators not only improve the quality of the final solutions but also significantly improve the convergence of the search process due to the use of feasible solutions. The results and effectiveness of the proposed technique are compared to the ones previously reported in the literature such as particle swarm optimizer, genetic algorithms and dynamic programming, among others.

13/00853 Solution of combined economic and emission dispatch problems of power systems by an opposition-based harmony search algorithm

Chatterjee, A. *et al. International Journal of Electrical Power & Energy Systems*, 2012, 39, (1), 9–20.

Evolutionary algorithms (EAs) are well-known optimization approaches to deal with non-linear and complex problems. However, these population-based algorithms are computationally expensive due to the slow nature of the evolutionary process. Harmony search (HS) is a derivative-free real parameter optimization algorithm. It draws inspiration from the musical improvisation process of searching for a perfect state of harmony. This paper proposes a novel approach to accelerate the HS algorithm. The proposed opposition-based HS of the present work employs opposition-based learning for harmony memory initialization and also for the generation jumping. In the present work, opposite numbers have been utilized to improve the convergence rate of the HS. The potential of the proposed algorithm, presented in this paper, is assessed by means of an extensive comparative study of the solution obtained for four standard combined economic and emission dispatch problems of power systems. The results obtained confirm the potential and effectiveness of the proposed algorithm compared to some other algorithms surfaced in the recent state-of-the-art literature. Both the near-optimality of the solution and the convergence speed of the proposed algorithm are found to be promising.

Economics, policy, supplies, forecasts

13/00854 Analyzing a micro-solid oxide fuel cell system by global energy balances

Meier, C. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10318–10327.

A simple method to predict the thermal characteristics of a micro-SOFC system is presented in this study. The basic design requirements for a thermally self-sustaining operation at a stack temperature of about 550 °C are assessed. Based on steady-state global energy and mass balances, the influence of the electrical efficiency, the overall air-to-fuel ratio and the heat losses on the operating temperature is discussed. It was found that at high electrical efficiencies and, hence, low heat release rates, a recuperator is needed to achieve the desired operating temperature. At lower electrical efficiencies, in contrast, disposing the released heat becomes an issue and an efficient cooling of the stack is required. Whether a recuperator or additional cooling components are necessary also depends on the electrical power output, the stack size and the thermal insulation specifications. The threshold between cooling and recuperator mode is of special interest, since this operating point allows a simple design of the thermal system without recuperator and only a minimum of air to be supplied to the system. This threshold efficiency, which is the maximal electrical efficiency that allows a thermally self-sustaining operation without recuperator, is above 50% under adiabatic operating conditions. In a non-adiabatic system, the threshold efficiency is reduced to about 45% in a 20 W_{el} and to about 20% in a 2.5 W_{el} system even with a state-of-the art thermal insulation. The considered thermal insulations dominate the system volume. Therefore, the ability of heat loss minimization is highly dependent on the targeted volumetric power density of the system.

13/00855 Application of SOM neural networks to short-term load forecasting: the Spanish electricity market case study

López, M. *et al. Electric Power Systems Research*, 2012, 91, 18–27.

The use of neural networks in load forecasting has been a popular research topic over the last decade. However, the use of Kohonen's self-organizing maps (SOM) for this purpose remains yet mostly unexplored. This paper presents a forecasting model based on this particular type of neural network. The scope of this study is not only to prove that SOM neural networks can be effectively used in load forecasting but to provide a deep and thorough analysis of the prediction and a real-world application. The data used to assess the validity of the model corresponds to Spain energy consumption from 2001 to 2010. Also meteorological data from this period has been used. The analysis comprises the study of the significance of different meteorological variables, the relevance of these meteorological data when recent load values are used as input and the effect of using different patterns to select the days to train the map. In addition, the evaluation of the frequency components of the data has provided an explanation to why apparently similar data sets allow different forecasting performances of the model. In order to build an application to the Spanish electricity market, the model was adjusted to timely forecast a load profile for each session of the daily and intra-daily markets. These forecasts are intended as an input to a decision support system for any commercializing company bidding on the market.

13/00856 Cost-saving potential of customer-driven distributed generation

Zeljković, Ć. and Rajaković, N. *Electric Power Systems Research*, 2012, 92, 87–95.

The focus of this research was to determine the realistically achievable cost-saving potential of customer-driven distributed generation. A novel real-time near-optimal algorithm for dispatching the customer DG units has been described and tested. The proposed method represents a powerful solution because the achievable savings almost reach the theoretical maxima, while the algorithm can be relatively easily implemented in automatic controllers. All the important input parameters have been included in the models, such as stochastically changeable load and meteorological parameters, non-linear DG cost curves, DG reliability issues, start-up costs, etc. Afterwards, the extensive simulations have been performed to determine which parameters are truly critical and which could possibly be idealized or completely ignored. The simulation results show that cost-saving potential of customer-driven DG is primarily dictated by the prices of fuel and electricity, i.e. their mutual ratio, as well as the deviation in customer load diagram. The value of DG is not significantly affected by the type of employed stochastic load model. Part-load decrease of DG efficiency is worth considering when the units dominantly operate at a peak-shaving mode. Although outages of DG units may sometimes noticeably deteriorate dispatch optimization for a particular month, the average results calculated for the real mean times to failure and repair show that DG reliability issues are not of a critical importance. Finally, it should be emphasized that the DG cost-saving potential and the performance index of the proposed dispatch algorithm are positively correlated. In case when an investment in DG is profitable due to a favourable ratio between the prices of fuel and electricity, both the performance of the algorithm and generation efficiency also achieve the highest values. On the other hand, the quality of the proposed dispatch strategy decreases in cases when DG investment is unprofitable either.

13/00857 Electric system management through hydrogen production – a market driven approach in the French context

Mansilla, C. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 10986–10991.

Hydrogen is usually presented as a promising energy carrier that has a major role to play in low carbon transportation, through the use of fuel cells. However, such a development is not expected in the short term. In the meantime, hydrogen may also contribute to reduce carbon emissions in diverse sectors among which methanol production. Methanol can be produced by combining carbon dioxide and hydrogen, hence facilitating carbon dioxide emission mitigation while providing a beneficial tool to manage the electric system, if hydrogen is produced by alkaline electrolysis operated in a variable way driven by the spot and balancing electricity markets. Such a concept is promoted by the VItESSE^2 project (INDUSTRIAL AND ENERGY value of CO_2 through Efficient use of CO_2-free electricity – Electricity Network System Control & Electricity Storage). Through the proposed market driven approach, hydrogen production offers a possibility to help managing the electric system, together with an opportunity to reduce hydrogen production costs.

13/00858 Electricity of Lebanon: problems and recommendations

Fardoun, F. *et al. Energy Procedia*, 2012, 19, 310–320.

This paper presents a detailed review of EDL (Electricité du Liban). It displays the institution's technical problems at the level of electricity generation, transmission and distribution as well as the administrative and financial states and suggests several recommendations. It is obvious that EDL suffers a great shortage in its generating capacity and human resources and would not be effective without conducting a national strategy that includes radical solutions.

13/00859 Energy network dispatch optimization under emergency of local energy shortage

Cai, T. *et al. Energy*, 2012, 42, (1), 132–145.

The consequence of short-time energy shortage under extreme conditions, such as earthquake, tsunami, and hurricane, may cause local areas to suffer from delayed rescues, widespread power outages, tremendous economic losses, and even public safety threats. In such urgent events of local energy shortage, agile energy dispatching through an effective energy transportation network, targeting the minimum energy recovery time, should be a top priority. In this paper, a novel methodology is developed for energy network dispatch optimization under emergency of local energy shortage, which includes four stages of work. First, emergency-area-centred energy network needs to be characterized, where the capacity, quantity, and availability of various energy sources are determined. Second, the energy initial situation under emergency conditions needs to be identified. Then, the energy dispatch optimization is conducted based on a developed MILP (mixed-integer linear programming) model in the third stage. Finally, the sensitivity of the minimum dispatch time with respect to uncertainty parameters is characterized by partitioning the entire space of uncertainty parameters into multiple subspaces. The efficacy of the developed methodology is demonstrated via a case study with in-depth discussions.

13/00860 Impact of inverter configuration on energy cost of grid-connected photovoltaic systems

He, F. *et al. Renewable Energy*, 2012, 41, 328–335.

This paper proposes a method to evaluate and optimize inverter configurations for grid-connected photovoltaic (PV) systems. It is studied by Monte-Carlo analysis that how the inverter configuration and its operation strategy would impact on lifetime energy yield and the levelized cost of energy (LCOE) considering the PV array scale, environmental conditions, system cost, inverter efficiency and reliability. The efficiency characteristic of parallel inverters with a common DC bus is deliberated along with the optimal operation strategy. Inverter system performance ratio (ISPR) is proposed as an overall index of lifetime energy conversion efficiency. A case study is performed to demonstrate the proposed method. It shows that the configuration with a common DC bus is a potential solution to reduce the energy cost of PV power generation systems. As ancillary results, it is found that optimizing the PV panel orientation can improve the probability distribution of solar irradiance on the panel, and it is confirmed that an oversized PV array may help reduce the energy cost.

13/00861 Predicting future hourly residential electrical consumption: a machine learning case study

Edwards, R. E. *et al. Energy and Buildings*, 2012, 49, 591–603.

Traditional whole building energy modelling suffers from several factors, including the large number of inputs required for building characterization, simplifying assumptions, and the gap between the as-designed and as-built building. Prior work has attempted to mitigate these problems by using sensor-based machine learning approaches to statistically model energy consumption, applying the techniques primarily to commercial building data, which makes use of hourly consumption data. It is unclear, however, whether these techniques can translate to residential buildings, since the energy usage patterns may vary significantly. Until now, most residential modelling research only had access to monthly electrical consumption data. This study reports on the evaluation of seven different machine learning algorithms applied to a new residential data set that contains sensor measurements collected every 15 min, with the objective of determining which techniques are most successful for predicting next hour residential building consumption. The authors first validate each learner's correctness on the ASHRAE great energy prediction shootout, confirming existing conclusions that neural network-based methods perform best on commercial buildings. However, the additional results show that these methods perform poorly on residential data, and that least squares support vector machines perform best – a technique not previously applied to this domain.

13/00862 Renewable electricity potentials in France: a long term perspective

Hubert, T. and Vidalenc, E. *Energy Procedia*, 2012, 20, 247–257.

Renewable energy sources play a role in providing energy services in a sustainable manner. This paper reviews and estimates the renewable electricity potentials in France in a long-term perspective, considering technical as well as social acceptability factors. Previous assessment studies are reviewed, and specific evaluations are conducted to estimate both the solar electricity potential on residential rooftops and the wind electricity potential in likely developable areas. Potential effects on the grid power balance are examined for typical winter and summer days based on historical data sets. France has the resources to produce a large portion of its annual final electricity consumption with renewable energy. However, further analysis is needed to evaluate more in depth the influence of limiting factors such as the variability of certain resources, the distribution and transmission constraints, and the potential usage conflicts.

13/00863 Sustainability and reliability assessment of microgrids in a regional electricity market

Prete, C. L. *et al. Energy*, 2012, 41, (1), 192–202.

This study develops a framework to assess and quantify the sustainability and reliability of different power production scenarios in a regional system, focusing on the interaction of microgrids with the existing transmission/distribution grid. The northwestern European electricity market (Belgium, France, Germany and the Netherlands) provides a relevant case study. Here, the authors present simulations of power market outcomes under various policies and levels of microgrid penetration, and evaluate them using a diverse set of metrics. This analysis is the first attempt to include exergy-based and reliability indices when evaluating the role of microgrids in regional power systems. The results suggest that a power network in which fossil-fuelled microgrids and a price on CO_2 emissions are included has the highest composite sustainability index.

13/00864 Various voltage productions by microbial fuel cells with sedimentary inocula taken from different sites in one freshwater lake

Song, T. S. *et al. Bioresource Technology*, 2012, 108, 65–75.

In this study, single-chamber microbial fuel cells (MFCs) were inoculated with sedimentary samples taken from one freshwater shallow lake. After 98 days of operation, it was found that sedimentary inocula had strong effect on MFC performances, and Fe(III) contents in sediments were significantly related to voltage values produced from MFCs. Inoculation of the sedimentary sample from the site with the highest Fe(III) content led to the production of the highest voltage with a value of 580 mV, while voltage from the MFC inoculated with sediments from the site with the lowest Fe(III) concentration was less than 30 mV at the end of the experiments. In addition, microbial communities of anode biofilms from the MFCs with the highest and lowest voltages showed significant difference. This study will help enable scientific decisions to be made regarding the selection of freshwater sediments as MFC inoculum, and survey exoelectrogenic microorganisms within sediments.

07 STEAM RAISING

Boiler operation/design

13/00865 Convective heat transfer in a mixture of cooling water and superheated steam

Kouhikamali, R. *et al. International Journal of Thermal Sciences*, 2012, 60, 205–211.

Desuperheaters are utilized to control the superheated steam temperature and provide a fine spray of cooling water in order to maximize the surface area for optimum evaporation process. One of the most important parameters in the modelling of desuperheaters that has to be considered is the effect of injected water quality on superheated steam temperature. Discrete phase model based on Eulerian–Lagrangian method that considered the Lagrangian approach for particle motion and the Eulerian approach for continuous phase is used to obtain the numerical results. In this article, the heat transfer of water droplets and the superheated steam is simulated as two-dimensional two-phase flow by considering k–ε turbulence modelling. The effects of water droplet diameter, vapour velocity and water mass flow rate on water evaporation rate and outlet steam temperature are investigated. Results show that the droplet diameter and superheated steam velocity have remarkable effect on the required length for evaporation of particles. Quantitative validation of the numerical model was implemented and the results showed a good agreement between numerical simulation and the experimental data taken from the literature.

13/00866 Evaluating the impact of an ammonia-based post-combustion CO_2 capture process on a steam power plant with different cooling water temperatures

Linnenberg, S. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 1–14.

The use of aqueous ammonia is a promising option to capture carbon dioxide from the flue gas of coal-fired power plants. Compared to a capture process using monoethanolamine (MEA), the use of ammonia can reduce the heat requirement of the CO_2 desorption significantly, although an additional effort is necessary to provide the cooling of the process. To allow for a fair evaluation of the integration of this CO_2 capture process into a power plant process, an overall process evaluation is carried out. The use of detailed models of the power plant, of the compressor and of the CO_2 capture process enables the calculation of the power loss due to the steam extraction as well as due to the required auxiliary power for CO_2 compression, solvent and cooling pumps and mechanical chillers. To study the influence of the cold end of the process, two power plants with different cooling water temperatures are analysed. Additionally, two different process configurations of the capture plant, with either one single absorber or two absorbers connected in series where the first absorber captures the majority of the CO_2 and the second limits the NH_3 slip, are evaluated. The influence of the main process parameters (desorber pressure, solvent circulation rate, solvent recycling rate and chilling temperature) are evaluated and the optimal configuration with respect to the overall net efficiency penalty is determined. The study shows that the configuration of the process with absorption at low temperature (approximately 10 °C) with or without precipitation of ammonium carbonate compounds leads to a lower net efficiency penalty than an

MEA-based process, assuming that low temperature cooling water is available. An estimate of the size of the absorber shows that the absorber columns of an ammonia-based process are significantly higher than the ones required for an MEA-based process.

13/00867 Further development of a microchannel steam reformer for diesel fuel

Maximini, M. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10125–10134.

This paper presents results from the on-going optimization of a microchannel steam reformer for diesel fuel which is developed in the framework of the development of a PEM fuel cell system for vehicular applications. Four downscaled reformers with different catalytic coatings of precious metal were operated in order to identify the most favourable catalyst formulation. Diesel surrogate was processed at varying temperatures and steam to carbon ratios (S/C). The reformer performance was investigated considering hydrogen yield, reformate composition, fuel conversion, and deactivation from carbon formation. Complete fuel conversion is obtained with several catalysts. One catalyst in particular is less susceptible to carbon formation and shows a high selectivity. To optimize the reformer geometry, a fifth downscaled reformer was implemented with an increased channel height. In operation the reformer shows advantages in performance and pressure losses in comparison to the original geometry.

13/00868 Optimal thermodynamic and economic volume of a heat recovery steam generator by constructal design

Norouzi, E. and Amidpour, M. *International Communications in Heat and Mass Transfer*, 2012, 39, (8), 1286–1292.

The ratios of gas flow to steam flow are huge in heat recovery steam generators (HRSGs) compared to other steam generators. So the volume which is occupied by components of the HRSG such as economizer, evaporator and superheater is important factor when the HRSG is applied in structures including buildings and ships. The optimum volume of a HRSG is deduced through optimization of entropy generation and cost evaluation. By increasing volume, second law of thermodynamics is improved, but this improvement may not be economical. In this work, the best dimensions and arrangements of flows in HRSG are obtained by constructal design and the optimization method is algorithm genetic. In this case, super heater temperature, pinch point, water/steam flow rate and gas pressure drop are derived from configuration which designed by constructal theory for HRSG. The effects of gas flow rate and inlet gas temperature are examined on the values of optimum volume.

13/00869 Particle emissions from a domestic pellets-fired boiler

Fernandes, U. and Costa, M. *Fuel Processing Technology*, 2012, 103, 51–56.

The main purpose of the present work was to quantify and characterize morphologically and chemically the emissions of particulate matter (PM) from a domestic pellet-fired boiler during steady-state operation for different boiler thermal inputs. The PM quantification was made with the aid of a low pressure three-stage cascade impactor and the PM characterization using SEM/EDS analysis (scanning electron microscope/energy dispersive X-ray spectrometry). The measured PM emissions varied between $\approx 160\,\mathrm{mg/N\,m^3}$@13% O_2 and $\approx 490\,\mathrm{mg/N\,m^3}$@13% O_2, being the emissions mainly dominated by particles with sizes below 2.5 µm and above 10 µm regardless of the thermal input. The SEM analyses revealed the presence of ultra-fine (<100 nm) particles, submicrometre- and micrometre-sized particles/agglomerates, and isolated spherical and irregularly shaped large particles for all boiler operating conditions examined. The ultra-fine particles, formed after the soot formation process, were composed mainly of O, K, Cl, Na and S; the submicrometre- (and micrometre)-sized particles/agglomerates, formed from soot, contained mainly carbon, oxygen, Ca, Mg, K and P; and the isolated spherical and irregularly shaped large particles, released from the fuel bed during combustion, consisted mostly of carbon and oxygen with minor amounts of Ca and Mg.

13/00870 Passivity degradation of nuclear steam generator tubing alloy induced by Pb contamination at high temperature

Lu, B. T. *et al. Journal of Nuclear Materials*, 2012, 429, (1–3), 305–314.

Effects of Pb contamination on the passivity of a Ni-based alloy (UNS N06690) in a simulated crevice chemistry of steam generator with near-neutral pH at 300 °C are elucidated using electrochemical measurements and surface analysis techniques. The experimental observations reveal that Pb impurity can enter anodic film, which results in substantial changes in the films structure via hindering the dehydration during the passivation and retarding the formation of spinel oxides. The presence of Pb-contamination can also increase hydrogen content in anodic film. Finally, the mechanism of passivity degradation induced by Pb contamination is described on the basis of the experimental data and established theory.

13/00871 Performance assessment for the water level control system in steam generator of the nuclear power plant

Zhang, Z. and Hu, L. S. *Annals of Nuclear Energy*, 2012, 45, 94–105.

The steam generator water level control system is the most important components of a nuclear power plant. The operating steam generator water level control system is increasingly recognized as a capital asset that should be routinely maintained and monitored. However, the control loop performance assessment is still an open problem; thus, the performance assessment technology will be brought into the steam generator water level control system in nuclear power plants. Performance assessment methods for the plant with stable and unstable zeros of two PI controller systems are developed at all specific power levels. The numerical examples will demonstrate the effectiveness of the proposed method.

13/00872 Steam oxidation of boron carbide–stainless steel liquid mixtures

Dominguez, C. *Journal of Nuclear Materials*, 2012, 427, (1–3), 140–151.

In the framework of nuclear reactor core meltdown accidents studies, the oxidation kinetics of boron carbide–stainless steel liquid mixtures exposed to argon/steam atmospheres was investigated at temperatures up to 1527 °C. A B–Cr–Si–O liquid protective layer forms on the surface of the mixtures in contact with steam. This protective layer gradually transforms into a Cr_2O_3-rich slag. Important quantities of liquid can be projected from the melt during oxidation. These projections are favoured by high B_4C contents in the melt, high steam partial pressures and low temperatures. In addition to stainless steel–boron carbide melts, simpler compositions (pure 304L stainless steel, iron–boron, iron–boron carbide and stainless steel–boron) were studied, in order to identify the basic oxidation mechanisms.

13/00873 Visualized investigation on flow regimes for vertical upward steam–water flow in a heated narrow rectangular channel

Wang, J. *et al. Annals of Nuclear Energy*, 2012, 45, 115–123.

Flow regimes are very important in understanding two-phase flow resistance and heat transfer characteristics. In this work, two-phase flow regimes for steam–water flows in a single-side heated narrow rectangular channel, having a width of 40 mm and a gap of 3 mm, were visually studied at relatively low pressure and low mass flux condition. The flow regimes observed in this experiment could be classified into bubbly, churn and annular flow. Slug flow was never observed at any of the conditions in this experiment. Flow regime maps at pressures of 0.7 and 1.0 MPa were developed, and then the pressure effect on flow regime transition was analysed. Based on the experimental results, the comparisons with some existing flow regime maps and transition criteria were conducted. The comparison results show that the bubbly transition boundary and annular formation boundary of heated steam–water flow were consistent with that of adiabatic air–water flow. However, the intermediate flow pattern between bubbly and annular flow was different. Hibiki and Mishima criteria could predict the bubbly transition boundary and annular formation boundary satisfactorily, but it poorly predicted churn zone in present experimental data.

08 COMBUSTION

Burners, combustion systems

13/00874 A comparative study on the pyrolysis of metal- and ash-enriched wood and the combustion properties of the gained char

Mayer, Z. A. *et al. Journal of Analytical and Applied Pyrolysis*, 2012, 96, 196–202.

This study aims to investigate the pyrolysis behaviour of metal-contaminated wood and the combustion properties of char derived from wood pyrolysis. Seven metals (Na, Mg, Ca, Zn, Cd, Pb and Fe(III)) were introduced to willow in cation form by ion-exchange and the thermal behaviour of demineralized samples and samples with additional ash were also investigated. The results show that the char yield increased from 21% to 24–28% and levoglucosan yield in vapour phase decreased from 88% to 62–29% after the addition of inorganic compounds, even though the metal binding capacity of wood varied from one metal ion to another. While char yield seems to be effected mainly by the concentration of the metal ions, levoglucosan yield was more dependent on the ionic species especially when sodium ions were present. When combustion experiments were carried out with char made of the metal enriched wood, two consecutive steps were observed, both effected by the presence of inorganic compounds. The first step was identified as the release and combustion of volatiles, while the second peak of the burning profile is the actual combustion of the fixed carbon. The burnout temperatures, estimated ignition indices and the conversion indicate that the type and not the amount of metal ions were the determining factors during the second step of combustion.

13/00875 A comparison of the emission and impingement heat transfer of LPG–H_2 and CH_4–H_2 premixed flames

Zhen, H. S. *et al. International Journal of Hydrogen Energy*, 2012, 37, (14), 10947–10955.

Experiments were performed to add hydrogen to liquefied petroleum gas (LPG) and methane (CH_4) to compare the emission and impingement heat transfer behaviours of the resultant LPG–H_2–air and CH_4–H_2–air flames. Results show that as the mole fraction of hydrogen in the fuel mixture was increased from 0% to 50% at equivalence ratio of 1 and Reynolds number of 1500 for both flames, there is an increase in the laminar burning speed, flame temperature and NO_x emission as well as a decrease in the CO emission. Also, as a result of the hydrogen addition and increased flame temperature, impingement heat transfer is enhanced. Comparison shows a more significant change in the laminar burning speed, temperature and CO/NO_x emissions in the CH_4 flames, indicating a stronger effect of hydrogen addition on a lighter hydrocarbon fuel. Comparison also shows that the CH_4 flame at $\alpha = 0\%$ has even better heat transfer than the LPG flame at $\alpha = 50\%$, because the longer CH_4 flame configures a wider wall jet layer, which significantly increases the integrated heat transfer rate.

13/00876 A new generalised model for liquid film cooling in rocket combustion chambers

Shine, S. R. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (19–20), 5065–5075.

A one-dimensional analytical model of liquid film cooling in rocket combustion chambers operating at subcritical conditions is developed. The approach followed involves the selection of a control volume for mass and energy balance. The coolant evaporation rate per area is obtained from this energy balance. The present model incorporates mass transfer via entrainment by adapting suitable correlations from literature pertaining to annular flow conditions. The model predicted favourably with the experimental data available in open literature and produced superior results compared to all existing models. Results are presented for a mixed gas–water system under different conditions. Results indicate that convection dominates the heat transfer at the gas–liquid interface. Effects of gas Reynolds number, coolant inlet temperature, combustion chamber pressure, mass flow ratio of the liquid coolant to the free stream and the free stream turbulence on the liquid film length are presented in detail.

13/00877 An Eulerian–Lagrangian computational model for deflagration and detonation of high explosives

Peterson, J. R. and Wight, C. A. *Combustion and Flame*, 2012, 159, (7), 2491–2499.

A solid phase explosives deflagration and detonation model capable of surface burning, convective bulk burning and detonation is formulated in the context of Eulerian–Lagrangian material mechanics. Well-validated combustion and detonation models, WSB and JWL++, are combined with two simple, experimentally indicated transition thresholds partitioning the three reaction regimes. Standard experiments are simulated, including the aluminium flyer plate test, the cylinder test, the rate stick test and the Steven test in order to validate the model. Cell and particle resolution dependence of simulation metrics are presented and global uncertainties assigned. Error quantification comparisons with experiments led to values generally below 7% (1σ). Finally, gas flow through porous media is implicated as the driving force behind the deflagration to detonation transition.

13/00878 Analysis of products from pyrolysis of Brazilian sugar cane straw

Moraes, M. S. A. *et al. Fuel Processing Technology*, 2012, 101, 35–43.

The main objective of this work is to investigate the chemical composition of the volatile compounds produced during the pyrolysis of sugar cane straw (SCS). The pyrolysis was conducted in a vertical furnace using a quartz reactor at a temperature of 700 °C (7 g of SCS, heating rate of 60 °C/min, flux of $1\,\mathrm{mL\,min^{-1}}$ of N_2 and 5 min of hold time at the final temperature). Pyrolysis products (solid residue and bio-oil) were analysed. The original biomass and the residual solid phase were characterized by thermogravimetric analysis (TGA) and infrared spectroscopy (FTIR). The biomass showed a TGA profile similar to cellulose and, according to FTIR analysis, it was rich in oxygenated compounds. The FTIR analysis of solid residue indicated that it was composed mainly by silica. Comprehensive two-dimensional gas-chromatography with time-of-flight mass spectrometry detector (GC × GC/TOFMS) was applied in the identification and semi-quantification of main compounds in bio-oil, allowing the identification of 123 compounds, mainly oxygenated (acids, ethers, aldehydes, ketones and phenols) with a predominance of furfural and hexenoic acid. The GC × GC/TOFMS allowed a group type classification of the compounds and a spatial organization that facilitated the identification of the main compounds in the two-dimensional diagram.

13/00879 Application of a particle model to pyrolysis. Comparison of different feedstock: plastic, tyre, coal and biomass

Navarro, M. V. *et al. Fuel Processing Technology*, 2012, 103, 1–8.

The thermal behaviour of solid particles of plastic, tyre, coal and biomass as feedstock in pyrolysis processes was studied. The samples were pyrolysed in a thermogravimetric analyser in nitrogen atmosphere (surface flow rate 2.65×10^{-3} m/s) at two different heating rates (5 and 10 °C/min) with temperatures ranging from 150 to 950 °C. This paper shows the successful application of the distributed energy model to study the effects of dynamic experiments on the solid pyrolysis, in particular, to ABS plastic and tyre rubber for the first time. In addition, the reaction model algorithm used was successfully implemented together with a heat transfer model to predict temperature profiles in the particle and to explore the effects of both solid characteristics and process conditions on the pyrolysis. Within the process conditions studied (particle size, inlet feedstock temperature, reactor temperature and global heat transfer coefficient) the particle size was the most influencing one. From the solid characteristics, the main influence in the particle behaviour was attributed to the characteristic devolatilization obtained in thermobalance showing the physicochemical properties a weak influence on it.

13/00880 Burner platform for sub-atmospheric pressure flame studies

Ombrello, T. *et al. Combustion and Flame*, 2012, 159, (7), 2363–2373.

Hencken burner flames at sub-atmospheric pressure were characterized experimentally to show their unique structure for detailed flame studies. Methane–air flames at 16.7 kPa were shown to be lifted and stably anchored at significant distances (up to 18 mm) above the burner surface, while maintaining a flat and one-dimensional laminar structure and near adiabatic conditions. Particle image velocimetry was used to identify the weakly stretched regime (strain rate = 20–$70\,\mathrm{s^{-1}}$) of the flames, as well as the flame speeds, while OH number densities were measured through laser-induced fluorescence and calibrated through absorption. The flame speeds and quantitative OH profiles were compared to one-dimensional and two-dimensional flame simulations using the chemical kinetic mechanisms of USC Mech II and GRI-3.0 and showed good agreement. Flames produced by a Hencken burner at sub-atmospheric pressure were shown to accurately represent a steady, laminar, nearly one-dimensional, minimally curved, weakly stretched, and near adiabatic flame, which could be compared to one-dimensional freely-propagating flame simulations with minimal corrections and extrapolations.

13/00881 Cold experiments on ligament formation for blast furnace slag granulation

Liu, J. *et al. Applied Thermal Engineering*, 2012, 40, 351–357.

Rotary cup atomization for molten slag granulation is an attractive alternative to water quenching. However, the mechanism of disintegration of molten slag must be assessed. In the present study, a glycerol/water mixture was substituted for molten slag, and the mechanism of ligament formation in a rotary cup was investigated using photos taken by a high-speed camera. The effects of the angular speed and inner depth of the rotary cup on ligament disintegration was investigated. The results showed that one state of disintegration may transform into another state as the angular speed of the rotary cup increases at a given liquid flow rate. During ligament formation, the number of ligaments increased with an increase in the angular speed of the rotary cup, and a decrease in the diameter of ligament and liquid drop was observed. Moreover, the initial point of disintegration of the ligament moved to the lip of the rotary cup as the angular speed increased. An equation describing the relationship between the diameter of the liquid drop and various factors was used to predict the diameter of the liquid drop. A rotary cup with an inner depth of 30 mm was the best choice for granulation. The results of the present study will be useful for designing devices used in molten slag granulation.

13/00882 Combustion properties of torrefied willow compared with bituminous coals

Jones, J. M. *et al. Fuel Processing Technology*, 2012, 101, 1–9.

Thermal pre-treatment, or torrefaction, is a process that can improve the handling and grinding properties of biomass for combustion and co-firing. This paper compares the combustion properties of raw and torrefied short rotation coppice (SRC) willow, with those of typical bituminous power station coals. The fuels were analysed using a number of standard fuel characterization tests. Willow SRC was torrefied at 290 °C for two reaction times (10 min (short) and 60 min (long)). During torrefaction, longer reaction time promotes loss of nitrogen from the solid product. Chars were produced from the fuels under high heating rates up to 1000 °C and the char yields and nitrogen partitioning were determined. Results show that the nitrogen partitioning for both raw and torrefied biomass favours release of nitrogen into the volatiles during rapid pyrolysis. In contrast, rapid pyrolysis of the coals favours nitrogen retention in the char. The chars were subjected to thermogravimetric analysis-mass spectrometry (TGA-MS) combustion tests, which were used to calculate the char reactivities and fate of char nitrogen. The char reactivities follow the order coal char < torrefied willow char < raw willow char. The release of volatile-nitrogen species during char combustion occurs at higher temperatures for the torrefied willow chars compared to the raw willow chars due to their relatively lower reactivities. Like coal char, nitrogen is concentrated in the char (both raw and torrefied willow chars) as combustion proceeds and NO and N_2 species are released towards the end of char burnout.

13/00883 Comparison of catalytic performance of Ag- and K-based catalysts for diesel soot combustion

Shimokawa, H. *et al. Catalysis Today*, 2012, 185, (1), 99–103.

Soot combustion performance of supported Ag (Ag/TiO_2 and Ag/CeO_2) and K (K/TiO_2 and K/CeO_2) catalysts under tight and loose contact conditions was evaluated by thermogravimetric analysis (TG) and the determination of the apparent activation energy as a function of soot conversion. The soot combustion performance strongly depended on the active species and contact conditions. The soot combustion proceeded by catalytic and non-catalytic combustion processes, depending on the contact conditions and the active species. Almost all the soot was catalytically combusted over Ag and K supported catalysts when they were tightly contacted with the soot, and Ag was more active catalytic species for soot oxidation than K. Under the loose contact condition, the supported K catalyst was superior to the supported Ag catalysts in the fraction of catalytically combusted soot and propagation of the combustion to the non-contact soot. Therefore, the supported K catalyst showed higher performance than the supported Ag catalyst for the removal of the majority of soot under the loose contact condition.

13/00884 Experimental research on inhibition performances of the sand-suspended colloid for coal spontaneous combustion

Xu, Y.-l. *et al. Safety Science*, 2012, 50, (4), 822–827.

Serious mine fire disasters have occurred in north-west China where there are abundant coal resources. For the shortage of water and loess, a large cost of conventional grouting slurry is needed. However, plenty of sand and fly ash resources have been found there. In order to improve the quality of sand injection and reduce the wastage of water during grouting, a kind of new compound material of sand-suspended colloid, which is composed of mineral inorganic gel and organic polymer, was developed in this paper. And the inhibition performance experiments of the sand-suspended colloid were carried out. The results show that the sand-suspended colloid efficaciously affected the oxidation characteristics above the critical temperature during the acceleration oxidation of the lignite and fat-gas coal samples and restrained the oxidation course by increasing the activation energy, so that it reduced the contents of CO and C_2H_4 and depressed the oxidation rate during the coal spontaneous combustion, and finally inhibited the coal spontaneous combustion.

13/00885 Experimental study and three-dimensional simulation of premixed hydrogen/air flame propagation in a closed duct

Xiao, H. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11466–11473.

An experimental and numerical study of premixed hydrogen/air flame propagation in a closed duct is presented. High-speed schlieren photography is used in the experiment to record the changes in flame shape and location. The pressure transient during the combustion is measured using a pressure transducer. A dynamic thickened flame model is applied to model the premixed combustion in the numerical simulation. The four stages of the flame dynamics observed in the experiment are well reproduced in the numerical simulation. The oscillations of the flame speed and pressure growth, induced by the pressure wave, indicate that the pressure wave plays an important role in the combustion dynamics. The predicted pressure dynamics in the numerical simulation is also in good agreement with that in the experiment. The close correspondence between the numerical simulation and experiment demonstrate that the TF approach is quite reliable for the study of premixed hydrogen/air flame propagation in the closed duct. It is shown that the flame wrinkling is important for the flame dynamics at the later stages.

13/00886 Experimental study on the fractal characteristic of methane explosion flame

Yi, Y. *et al. Safety Science*, 2012, 50, (4), 679–683.

In this paper flame microstructures and propagation characteristic of methane explosion are studied by high speed schlieren photography technique. By experiment it shows that flame front surface and inner flow field of methane explosion has distinctly fractal characteristic, the effect of the wrinkle of flame front surface and inner reactants on flame propagation can be directly reflect by fractal dimensions. Fractal dimension has a direct relation to flame structure and flame propagation characteristics, and it is the important parameter to scale the flame propagation velocity and flame temperature.

13/00887 Flow characterisation of diffusion flame in a standing wave

Chen, L. W. *et al. Experimental Thermal and Fluid Science*, 2012, 41, 84–93.

The flow structure of acoustic standing wave and the interaction between the standing wave and a diffusion flame inside a square tube has been investigated using phase-locked particle image velocimetry (PIV) and high-speed schlieren visualization. The acoustic field induced by standing waves in a tube at different phases and its effect on both cold jet fuel flow and jet flame are measured and analysed. It is observed that the jet flow is a strong function of the phase angle. The acoustic field and flame properties at the different positions of the acoustically driven tube have been investigated. It is shown that both the cold fuel jet flow and the jet flame are highly sensitive to the location of standing wave in the tube. In the velocity node area, the jet is less affected by the excitation. In contrast, the jet was observed to experience large velocity variation in the velocity anti-node area. It can be seen that both the fuel flow and the ambient air are strongly affected by the acoustic excitation, and the coupling effect creates complex flame dynamics.

13/00888 Influence of turbulence–radiation interactions in laboratory-scale methane pool fires

Consalvi, J. L. *International Journal of Thermal Sciences*, 2012, 60, 122–130.

The objective of this study is to assess the effects of turbulence–radiation interactions (TRI) on the structure of small-scale pool fires and on the radiative fluxes transferred to surrounding surfaces. Fire-induced flow is modelled by using a buoyancy-modified k–ε model and the steady laminar flamelet (SLF) model coupled with a presumed probability density function (pdf) approach. A 34-kW methane pool fire produced by burner with a diameter of 0.38 m is simulated by neglecting radiation, by considering radiation without TRIs, and by considering radiation with TRIs. Computations carried out with radiation are based on the full spectrum correlated-k method. TRIs are taken into account by considering the Optically-thin fluctuation approximation. The mean radiative source term and the mean RTE are then closed by using a presumed pdf of the mixture fraction, scalar dissipation rate, and enthalpy defect. When TRIs are considered predicted flame structure, radiant fraction and radiative fluxes are found in quantitative agreement with the available experimental data. Simulations reveal that TRIs significantly enhance radiative losses and substantially contribute to the drop in temperature due to radiation. TRIs also contribute to reduce turbulence levels and the root mean square values of temperature fluctuations. In addition radiative heat fluxes on remote targets are found to be considerably higher than those obtained from radiative calculations based on mean properties. Finally different levels of closure for the TRI-related terms are assessed. Model results show that the complete absorption coefficient-Planck function correlation should be considered in order to properly take into account the influence of TRIs on the emission term whereas the effect of absorption coefficient self-correlation on the absorption term is a reduction by about 12% of the radiant fraction.

13/00889 Kinetic study of the combustion of ethanol and ethyl acetate mixtures over a MnCu catalyst

Campesi, M. A. *et al. Fuel Processing Technology*, 2012, 103, 84–90.

A kinetic study of ethanol and ethyl acetate combustion on an efficient catalyst identified as Mn_9Cu_1 is reported in this contribution. Ethanol and ethyl acetate are typical VOCs which can be found in effluents of printing industries. Ethanol oxidation produces an intermediate product, acetaldehyde. On the other hand, ethyl acetate oxidation produces directly CO_2 and H_2O. Acetaldehyde reacts more slowly than ethanol, while ethyl acetate is slightly more difficult to oxidize than acetaldehyde. Strong inhibition effects among the species involved (ethanol, ethyl acetate and acetaldehyde) should be explicitly considered to propose reaction rate expressions. Thus, experimental data were satisfactorily fitted employing LHHW type expressions. The estimated activation energy of ethyl acetate and ethanol oxidation lies in the range of values reported in the literature for similar catalysts.

13/00890 Pd–Pt bimetallic catalysts for combustion of SOFC stack flue gas

Hoque, Md. A. *et al. Catalysis Today*, 2012, 185, (1), 66–72.

Pd–Pt bimetallic as well as monometallic Pd and Pt catalysts were evaluated to study the catalyst activity and stability for combustion of SOFC stack flue gas. The simulated reactant gases consisting of H_2, CO, CH_4, air and water vapour were tested at two different GHSV for obtaining the behaviour of catalyst activity versus temperature and catalyst stability versus on-stream operation hours. As H_2 and CO were readily combusted under 200 °C and CH_4 was combusted only above 300 °C, catalyst activity was evaluated by measuring CH_4 conversion as a function of temperature for all five catalysts. Catalyst stability was evaluated by monitoring CH_4 conversion for 1:1 Pd–Pt and 1:3 Pd–Pt catalysts exhibiting relatively better activity at 427 and 627 °C for 200 h. 1:1 Pd–Pt catalyst was the most active one based on the lowest CH_4 light-off temperature and the lowest temperature for complete CH_4 conversion, and this catalyst was deactivated less than 1:3 Pd–Pt catalyst in the 200 h-stability test. 1:1 Pd–Pt composition was attributed as the synergistic factor of active metal ingredients affecting the catalyst activity and stability. The presence of water vapour in the reactant gas inhibited catalyst activity and stability strongly by forming some less or inactive palladium species on catalyst surface via interaction between water molecules and catalyst active sites.

13/00891 Predicting the pyrolysis of single biomass particles based on a time and space integral method

Haseli, Y. *et al. Journal of Analytical and Applied Pyrolysis*, 2012, 96, 126–138.

The objective of this paper is to present a simple pyrolysis model to capture the main characteristics of the decomposition of a thermally thin particle at high temperatures corresponding to those found in the furnace of coal/biomass power plants. To achieve this goal, it is assumed that pyrolysis begins soon after the surface of the particle has reached a certain pyrolysis temperature, and proceeds according to a shrinking (unreacted) core model with an infinitesimal reaction front. The formulation of various stages including initial heating, pre-pyrolysis heating, pyrolysis and post-pyrolysis heating is carried out based on a time and space integral method which allows one to describe the energy conservation equation in an algebraic form. Two different treatments are presented for the pyrolysis stage. The first formulation assumes separate temperature profiles for char and biomass regions (double-temperature profile), whereas in the second treatment only one profile is considered for the temperature throughout the particle (single-temperature profile). Of particular interest is the latter approach that leads to simple relationships for predicting the duration of various stages, enabling one to predict the mass loss history. The accuracy of both methods is examined by comparing their predictions with recent experimental data reported in the literature as well as the prediction of comprehensive pyrolysis models. Satisfactory agreement is achieved indicating that both pyrolysis models based on double- and single-temperature profiles can be used with sufficient accuracy for engineering purposes.

13/00892 Pressurized chemical-looping combustion of coal using an iron ore as oxygen carrier in a pilot-scale unit

Xiao, R. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 363–373.

Chemical looping combustion (CLC) of coal is established as a new concept for inherent CO_2 separation with the advantages of low cost and high conversion efficiency. A pilot-scale unit consisting of two fluidized bed reactors was constructed and operated to study the performance of pressurized chemical-looping combustion (PCLC). Experiments were conducted using Shenhua bituminous coal as fuel and MAC iron ore as oxygen carrier at three different operation pressures (0.1, 0.3 and 0.5 MPa) and the unit has been operated for totally 19 h with steady coal-feeding, about 13.5 h of which were realized under stable operation. The results showed that PCLC of coal demonstrated many remarkable advantages over the conventional CLC of coal, in terms of the improvement of carbon conversion in the fuel reactor, CO_2 concentration of exhaust gas and combustion efficiency. At the operating pressure of 0.5 MPa, the CO_2 concentration, carbon conversion and combustion efficiency reached very high values of 97.2, 84.7 and 95.5% respectively. The potential of low-cost iron ore as oxygen carrier for commercial coal-fuelled CLC unit was also examined. The loss of oxygen carrier due to fine particles leaving the reactors increased with the increase of operation pressure and no agglomeration of oxygen carrier particles occurred during these tests. The oxygen carrier used in PCLC tests were also characterized by SEM-EDX and BET analysis to further emphasis on the effects of operation pressures and runtime.

13/00893 Rapid co-pyrolysis of rice straw and a bituminous coal in a high-frequency furnace and gasification of the residual char

Yuan, S. *et al. Bioresource Technology*, 2012, 109, 188–197.

Rapid pyrolysis of rice straw (RS) and Shenfu bituminous coal (SB) separately, and rapid co-pyrolysis of RS/SB blends (mass ratio 1:4, 1:4, and 4:1), were carried out in a high-frequency furnace which can ensure both high heating rate and satisfying contact of fuel particles. Synergies between RS and SB during rapid co-pyrolysis were investigated. Intrinsic and morphological structures of residual char from co-pyrolysis, and their effects on gasification characteristics were also studied. Synergies occurred during rapid co-pyrolysis of RS and SB (RS/SB = 1:4) resulting in decreasing char yields and increasing volatile yields. Synergies also happened during gasification of the char derived from co-pyrolysis of RS and SB with mass ratio of 1:4. The increased mass ratio of RS to SB did not only weaken synergies during co-pyrolysis, but significantly reduced the gasification rates of the co-pyrolysis char compared to the calculated values.

13/00894 Release of offensive odorants from the combustion of barbecue charcoals

Rahman, M. M. and Kim, K. H. *Journal of Hazardous Materials*, 2012, 215–216, 233–242.

A number of offensive odorants including volatile organic compounds (VOCs), reduced sulfur compounds (RSCs), carbonyls, and ammonia were measured along with several reference pollutants (like benzene (B), CS_2, SO_2, CO, and total hydrocarbon (THC)) from combusted fumes of barbecue charcoals produced from five different countries (Korea, China, Indonesia, Malaysia and the USA). Although the emission concentrations of most odorants were generally below the reference guideline set by the malodour prevention law in Korea, the mean concentration of some aldehydes (acetaldehyde, propionaldehyde, and isovaleraldehyde) and ammonia exceeded those guidelines. As such, aldehydes were the most dominant odorant released from charcoal combustion followed by VOC and ammonia. If odorant levels of charcoal products are compared, there are great distinctions between the products of different countries. If comparison is made using the concept of the sum of odour intensity, the magnitude of SOI for the charcoal products from the five different countries varied in the order of 4.30 (Korea), 3.10 (Indonesia), 2.97 (China), 2.76 (Malaysia), and 2.76 (USA).

13/00895 Research and application of comprehensive electromagnetic detection technique in spontaneous combustion area of coalfields

Shi, X.-x. *Safety Science*, 2012, 50, (4), 655–659.

Perplexed by severe disasters, spontaneous combustion areas of coalfields in China not only lose a large number of precious coal resources but damage the ecological environment badly. The premise of effective control against the disasters is investigations on the source position and scope of spontaneous combustion areas at coalfields so as to provide scientific basis for fire extinguishment design and construction of coalfields. Working principles, construction methods and detection effects of high resolution earth resistivity method, transient electromagnetic method (small loop-centre probe device) applied in the detection of combustion areas at coalfields have been introduced. The application shows that the above mentioned methods can detect the accurate position of underground combustion areas, are effective ones in detecting the combustion centre, combusted area and distribution scope of combustion areas at coalfields, and have broad application prospects.

13/00896 Supported manganese dioxide catalyst for seawater flue gas desulfurization application

Bian, J. *et al. Chemical Engineering Journal*, 2012, 189–190, 57–61.

In seawater flue gas desulfurization (FGD) process, ceramic supported MnO_x catalysts were developed to improve SO_2 removal efficiency of the scrubber by increasing S(IV) oxidation rate at the low pH values. These supported MnO_x catalysts were prepared by impregnation–precipitation method, calcined at different temperatures, and exposed to simulated flue gases to investigate the catalytic oxidation of sulfur dioxide in seawater buffering system. Compared with 'blank' ceramic, the most active MnO_x/ceramic catalyst, 623MnO_x/ceramic, that was prepared by doping $(NH_4)_2CO_3$ as the precipitant and calcined at 623 K, exhibited up to 17% higher SO_2 conversion at the GHSV 3000 h^{-1} in the industrial feasible temperature range of 318–358 K. XPS spectra revealed manganese was in the state of oxidation +4 on the surface of 623MnO_x/ceramic. XRD patterns and SEM-EDS spectra indicated that the high activity of 623MnO_x/ceramic for S(IV) oxidation at low temperatures could be attributed to oxygen activation and transfer ability of highly dispersed MnO_2 on ceramic support. H_2-TPR profiles showed the low temperature reduction peak was shifted to higher temperature when the calcination temperature increased from 573 to 723 K, and low temperature reducible manganese species were related to catalytic activity for S(IV) oxidation. The good performance of MnO_2/ceramic catalyst on the SO_2 removal appeared to be promising in seawater FGD application when high-sulfur coals were burned.

13/00897 The effect of temperature on the condensed phases formed in fuel-rich premixed benzene flames

Russo, C. *et al. Combustion and Flame*, 2012, 159, (7), 2233–2242.

The sooting structure of premixed fuel-rich atmospheric pressure benzene flames burning at the same C/O molar ratio = 0.8 was studied in different temperature conditions ($T_{\max} = 1720\,\mathrm{K}$ and 1810 K) by changing the cold gas velocity. Compositional profiles of gaseous and condensed phases, measured by probe sampling and chemical analysis, indicated that pyrolytic routes leading to higher soot formation are more favoured in the lower temperature conditions. The structural analysis of condensed phases, including condensed species and soot, has been carried out by using FT-IR and UV–visible spectroscopy sensitive to the hydrogen bonding and carbon network, respectively. The very low hydrogenated character, as evaluated by FT-IR and elemental analysis, and the high aromatic/graphitic nature of the benzene soot, as shown by a detailed examination of UV–visible spectral parameters, confirmed the effect of benzene fuel on the internal structure of soot particles already in the early stages of particle inception.

13/00898 The relationship between oxygen consumption rate and temperature during coal spontaneous combustion

Zhu, J. *et al. Safety Science*, 2012, 50, (4), 842–845.

Spontaneous combustion is a major natural disaster in coal production. In the process of exploring coal self-ignition, a series of hypotheses have been put forward, most scholars agree that the current coal–oxygen compound theory. Oxygen consumption rate reflects the status of coal spontaneous combustion, and it is also one of the parameters necessary for numerical simulation of coal spontaneous combustion. In this paper, a coal heating and oxidation experiment was designed, Experimental device consists of heating and oxidation furnace, gas chromatograph, temperature control and data acquisition systems and other equipment components. Three coal samples whose weight each is 5 g were selected for the study. By experiment, oxygen concentration at the inlet and outlet of temperature oxidation furnace was measured. Oxygen consumption rate is calculated in the heating process of coal according to air flow. In the Cartesian coordinate system, the temperature as abscissa and the oxygen consumption rate for the longitudinal coordinates, drawing the relationship between oxygen consumption rate and temperature plot. And then regression analysis was used to analyse the relationship between oxygen consumption rate and coal temperature during the heating and oxidation process of coal. The results show that the oxygen consumption rate and temperature of coal were linear relationships both before and after the critical temperature when the coal temperature is less than 180 °C. Before the critical temperature oxygen consumption rate is low, however it increases rapidly when coal temperature reaches a critical temperature. The result is important for the prevention and treatment of spontaneous combustion of coal.

13/00899 Thermogravimetric–mass spectrometric analysis of lignocellulosic and marine biomass pyrolysis

Sanchez-Silva, L. *et al. Bioresource Technology*, 2012, 109, 163–172.

The pyrolysis characteristics of three lignocellulosic biomasses (fir wood, eucalyptus and pine bark) and a marine biomass (*Nannochloropsis gaditana* microalgae) were investigated by thermogravimetric analysis coupled with mass spectrometry (TGA–MS). Thermal degradation of lignocellulosic biomass was divided into four zones, corresponding to the decomposition of their main components (cellulose, hemicellulose and lignin) and a first step associated to water removal. Differences in volatile matter and cellulose content of lignocellulosic species resulted in different degradation rates. Microalgae pyrolysis occurred in three stages due to the main components of them (proteins), which are greatly different from lignocellulosic biomass. Heating rate effect was also studied. The main gaseous products formed were CO_2, light hydrocarbons and H_2O. H_2 was detected at high temperatures, being associated to secondary reactions (char self-gasification). Pyrolysis kinetics were studied using a multiple-step model. The proposed model successfully predicted the pyrolytic behaviour of these samples resulting to be statistically meaningful.

13/00900 Transition characteristics of combustion modes for flame spread in solid fuel tube

Matsuoka, T. *et al. Combustion and Flame*, 2012, 159, (7), 2466–2473.

This paper provides a new concept based on the Damköhler number (*Da*) to describe the complete transition behaviour found in a flame spread in a solid combustible tube. Through a series of experiments performed with various diameters of the tube, ambient pressure, and oxidizer velocity within a wide range, three combustion modes are observed for the flame spread in a solid fuel tube, namely combustion dominated by heat transfer (mode 1), by chemical kinetics (mode 2), and slow combustion sustained under very high blowing conditions (so-called ‘stabilized combustion’: mode 3). Previous studies on the flame spread in tubes have shown that each transition, from mode 1 to mode 2 (transition 1–2) and from mode 2 to mode 3 (transition 2–3), is characterized by an equivalent velocity and by a friction velocity respectively. Meanwhile, for a flame spread on a fuel plate, it is widely known that both transitions are summarized by the *Da*. To achieve a comprehensive understanding of the transition characteristics of the combustion modes for the flame spread in the tube, the flame-spread rates under various conditions are experimentally investigated to elucidate the parameters that determine both transitions. First, the authors introduce a laminar friction velocity for the laminar flow region and revealed that transition 2–3 is determined by the laminar and turbulent friction velocity for laminar flow and turbulent flow regime respectively. The correlation between the *Da* and the friction velocity was experimentally obtained to show that transition 2–3 is consequently determined by the *Da*. This finding suggests that transition 2–3 corresponds to a blow-off limit that is observed for flame spread on a fuel plate. Second, the same correlation between the non-dimensional flame-spread rate and the *Da* is obtained, and it clearly showed that the transition 1–2 was determined by the *Da*. In conclusion, both transition phenomena are physically identical to those observed for on-plate flame spread, except the transition 2–3 occurs instead of the blow-off.

Fire safety

13/00901 Analysis of the Schiphol Cell Complex fire using a Bayesian belief net based model

Hanea, D. M. *et al. Reliability Engineering & System Safety*, 2012, 100, 115–124.

On the night of 26 and 27 October 2005, a fire broke out in the K-wing of the Schiphol Cell Complex near Amsterdam, the Netherlands. Eleven of 43 occupants of this wing died due to smoke inhalation. The Dutch safety board analysed the fire and released a report 1 year later. This article presents how a probabilistic model based on Bayesian networks can be used to analyse such a fire. The paper emphasizes the usefulness of the model for this analysis. In additional it discusses the applicability for prioritization of the recommendations such as those posed by the investigation board for the improvements of fire safety in special buildings. The big advantage of the model is that it can be used not only for fire analyses after accidents, but also prior to the accident, for example in the design phase of the building, to estimate the outcome of a possible fire given different possible scenarios. This contribution shows that if such a model was used before the fire occurred the number of fatalities would have not come as a surprise, since the model predicts a larger percentage of people dying than happened in the real fire.

13/00902 Change in activity of catalysts for the oxidation of tritium during a fire event

Iwai, Y. *et al. Fusion Engineering and Design*, 2012, 87, (7–8), 946–950.

The catalytic performance should be maintained in any off normal events. Fire accident is the typical off normal event. In the fusion plant, typical combustibles are evaluated to be polymeric low-halogen cables. Produced gases from burned low-halogen cable may affect the activity of catalysts for the oxidation of tritium. The authors experimentally demonstrated the influence of produced gases from burned low-halogen cable on the activity of catalyst using tritium gas. This evaluation showed that ethylene, methane and benzene were major produced gases. The activity of catalysts for the oxidation of tritium during a fire event was evaluated using a commercial hydrophilic Pt/Al_2O_3 catalyst and a commercial hydrophobic Pt-catalyst. The temperature of catalytic reactor was selected to be 423 and 293 K. At 423 K, no considerable decrease in catalytic activity was observed for both catalysts even in the presence of produced gases from burned low-halogen cable. At 293 K, considerable increase in catalytic activity was initially observed for both catalysts due to the effect of produced hydrogen. Then the temporary decrease was observed, however the catalytic activity was gradually recovered to be the original activity. Consequently, the irreversible decrease in activity of the catalysts during a fire event was not observed.

13/00903 Dynamic numerical simulation of coal mine fire for escape capsule installation

Zhang, S. *et al. Safety Science*, 2012, 50, (4), 600–606.

A fire in a mine laneway leads to disordered ventilation system airflow, and the smoke will result in staff poisoning. In such situation, it is necessary to install a rescue capsule in the common staff area. In this paper, the software Fluent was used to simulate the airflow conditions dynamically in No. 5 belt roadway of the Kongzhuang coal mine when fire broke out. The migration law of the CO front was determined. By underground escape experiments, a personnel escape velocity model in pathway was established. Based on the numerical simulation and results of field experiments, the escape capsule installation location in the passageway of No. 5 belt roadway was ascertained.

13/00904 Effects of slope on fire spread observed through video images and multiple-point thermal measurements

Silvani, X. *et al. Experimental Thermal and Fluid Science*, 2012, 41, 99–111.

A series of nine fire experiments was conducted on a large-scale bench with an inclinable plate to study the effects of a slope on fire spread. The temperature and total and radiant heat flux densities were measured at the top of the fuel bed during the upslope fire spread in still air. Measurements were recorded at five different locations ahead of the fire front. The effects of the slope on the flame topology, fire dynamics, and heat transfers ahead of the fire front were observed. The thermal measurements and image analyses showed a change in the fire spread regime and its related behaviour with an increase in the slope. This was observed through an elongation of the flame and its contact surface over the upper part of the fuel bed. When the slope increased, the fire topology changed from a U-shape to a V-shape, and the radiation-dominated thermal environment ahead of the flame front was progressively turned into a mixed convective-radiative one, in which convection finally dominated for steep slope configurations. For fire spreading across a 30° slope, this increase in the curvature of the fire front (V-shape) is associated with the appearance of fire whirls rolling along the flanks of the fire front, which indicates significant changes in the fluid mechanics and heat transfers. The span of the heat transfer increased and a significant amount of energy impinged 1 or 2 m ahead of the flame front because of the flame tilt (radiation) and hot gas flow (convection). The measurements also indicated a greater amount of energy impinging in the centre of the fuel bed than at the edge. This study shows the importance of investigating the fluid mechanics of fire in future wildfire researches.

13/00905 Experimental investigation on influence of different transverse fire locations on maximum smoke temperature under the tunnel ceiling

Ji, J. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4817–4826.

In former studies, fires were always assumed to occur at the longitudinal centreline of tunnels. In fact, fires will occur at any locations in tunnels, with different distances to the sidewall. A set of model scale experiments were carried out, to investigate the influence of different transverse fire locations on maximum smoke temperature under the tunnel ceiling. Results show that the restriction effect of the sidewalls of tunnels cause the maximum smoke temperature rise under the ceiling to increase compared with the unconfined space, even fires occurs at the longitudinal centreline. The maximum smoke temperature rises above the fire keep almost unchanged with the fire moving closer to the sidewall at the beginning and then increase significantly after the distance between the fire and the sidewall decreases to a certain value. For small pools of wall fire, the ‘mirror’ effect is reasonable, and for large pools, will bring a relatively large error without considering the influence of the equivalent diameter of a wall fire, resulting in underestimating the mass flow rate of fire plume and then overestimating the smoke temperature. Under all fires, the maximum smoke temperature rise under the ceiling decreases exponentially as the longitudinal distance from fire increases. Correlations for related parameters are proposed.

13/00906 Experimental research on thermal stratification of liquefied gas in tanks under external thermal attack

Shi, J. *et al. Experimental Thermal and Fluid Science*, 2012, 41, 77–83.

When liquefied gas tanks are exposed to fire, the temperature and pressure in tanks will increase and may cause boiling liquid expanding vapour explosion (BLEVE). According to relevant researches, the likelihood and the severity of BLEVE’s hazards are significantly affected by the thermal stratification of liquefied gas. In this research, a device was set up to simulate the thermal response of liquefied gas tank under external thermal attack. In the tests two uniform electric heaters were used to simulate the fire, and a small steel vessel was used to simulate the tank, and the liquefied gas was simulated by water. The fill level, the heater power and the heated area were adjusted in the tests to simulate different accident conditions. The results showed that the liquid temperature is nearly uniform when the liquid space wall was heated solely; however, the temperature stratification was obvious when the liquid and vapour space walls were heated simultaneously. Based on the experimental results, this paper discusses how the temperature stratification appears and fades away.

13/00907 Fire-ball expansion and subsequent shock wave propagation from explosives detonation

Kwak, H. Y. *et al. International Journal of Thermal Sciences*, 2012, 59, 9–16.

A well-known problem in thermo-hydrodynamics involves the sudden release of the explosion energy, concentrated in a finite volume, to surroundings with uniform density. However, only similarity solutions which have no detailed information on the earlier behaviour of the fire-ball are available on this problem. This study obtained a set of analytical solutions for the time dependent radius of an expanding fire-ball after explosives detonation by solving continuity, Euler and energy equations using a ‘polytrope’ assumption for the fire-ball centre. Subsequent spherical shock waves that develop from the fire-ball are obtained using the Kirkwood–Bethe hypothesis with Tait’s equation of state for water and the ideal gas equation of state for air. The pressure waves emanating from the oscillating bubble in underwater, which has a notably different time scale from the shock wave generation, are obtained using the Rayleigh equation. The calculated results for the period and the maximum radius of bubble that resulted from the fire-ball and the pressure wave from the oscillating bubble in underwater are similar to observed ones. The calculated peak pressures as a function of shock radius in air medium were comparable to those observed.

13/00908 Highly responsive hydrogen gas sensing by partially reduced graphite oxide thin films at room temperature

Wang, J. *et al. Carbon*, 2012, 50, (11), 4061–4067.

Novel chemo-resistive gas sensors based on reduced graphite oxide (rGO) thin films have been fabricated and evaluated for hydrogen detection. The rGO materials were thermally treated at various conditions and analysed using X-ray diffraction, Fourier transform infrared spectroscopy, and X-ray photoelectron spectroscopy techniques to investigate the change of functional groups. The semiconductor type of the rGOs treated at different conditions were checked by flowing hydrogen gas at 20 cm^3/min (sccm) under 10 Torr partial pressure. The rGOs treated at 70 °C in atmosphere (rGO070a), 200 °C in a vacuum (rGO200v), and 500 °C in a vacuum (rGO500v) exhibited n-type, ambipolar, and p-type behaviour, respectively. The rGO500v was adopted as active sensing element without any rare metal decoration, and its sensing response to hydrogen was studied by using air as carrier gas. The rGO500v exhibited good sensitivity (~4.5%), response time (~20 s), and recovery time (~10 s) to 160 ppm hydrogen gas at room temperature.

13/00909 Numerical simulation of premixed methane–air deflagration in large *L/D* closed pipes

Bi, M. *et al. Applied Thermal Engineering*, 2012, 40, 337–342.

A three-dimensional numerical model in which the heat loss through pipe walls was included was developed to simulate gaseous deflagration in pipes of large length-to-diameter ratio (L/D). The simulated pressure time histories are in good agreement with published data, and the error between experimental and computed maximum pressure is less than 15.3%. The attention is focused on the flame propagation and flow field during deflagrations, as well as the effects of ignition point (at the centre or at one end of the pipe) and L/D ($L/D = 6 - 10.35$) of the pipe on them. The numerical results show that a tulip flame is formed during flame propagation, which is related to the reverse flow and vortices motion. The maximum fame speed is 30% higher with the ignition point at the end than that at the centre, and it increases linearly with increasing L/D. The deflagration pressure decreases when the distance that flame travels increases due to the effect of the heat loss through pipe walls.

13/00910 Prediction of the mass loss rate of polymer materials: impact of residue formation

Kempel, F. *et al. Combustion and Flame*, 2012, 159, (9), 2974–2984.

Two different numerical simulation tools, fire dynamic simulator (FDS) and ThermaKin, are investigated with respect to their capability to predict the mass loss rate of polymer materials exposed to different fires. For validation, gasification apparatus and cone calorimeter tests are conducted. The main focus is on the influence of residue formation. Therefore, poly (butylene terephthalate) (PBT) and PBT reinforced with glass fibres (PBT-GF) are investigated and compared. PBT decomposes almost completely, while PBT-GF forms residue. The materials are characterized in order to provide suitable input parameters. Additionally the total incident heat flux to the sample is measured. With accurate input parameters, FDS and ThermaKin predicted the pyrolysis behaviour of PBT very well. Only some limitations are identified regarding the residue-forming PBT-GF. Both numerical simulation tools demonstrate a high value regarding the assessment of parameters’ relative impacts and thus the evaluation of optimization routes in polymer and composite development.

13/00911 Sensors for the ultra-fast monitoring of explosive gas concentrations

Vasiliev, A. A. and Malyshev, V. V. *Procedia Engineering*, 2012, 47, 224–227.

The target of this paper is answering the question about the minimum response time of metal oxide semiconductor gas sensors. This question is very important at the monitoring of sudden explosive emission of high concentrations of combustible gases in mines, chemical and oil refinery factories, nuclear power stations, etc. The optimization of the thickness of sensing layer, deposition conditions, material, and working temperature enabled the fabrication of the sensor with very short response time ~160 ms (hexane) in a concentration range up to 12 vol. %. The response time of the sensor was compared with the response time of IR optic sensor based on LED ($\lambda = 3.4$ micron) using testing gas mixing installation equipped with ultra-fast valves. The results were proven in field experiment with spike emission of petrol aerosol.

13/00912 The influence of diaphragm rupture rate on spontaneous self-ignition of pressurized hydrogen: experimental investigation

Golovastov, S. and Bocharnikov, V. *International Journal of Hydrogen Energy*, 2012, 37, (14), 10956–10962.

Influence of rupturing process on a diffusion self-ignition of hydrogen was studied experimentally at a pulse discharge into an open channel filled with air. Self-ignition of hydrogen occurred at a contact surface of the jet of hydrogen. Required temperatures for self-ignition were reached due to heating the air by a shock wave which appears as a result of the non-stationary discharge of hydrogen from the high pressure vessel. Initial pressure of hydrogen was varied from 3 to 14 MPa. Rupture duration of a diaphragm was measured. Rupture rate of the diaphragm was determined by an intensity of light, passing through the diaphragm. Formation of a shock wave flow structure at the pulse discharge of compressed hydrogen into the channel with air was studied, and ignition delays of hydrogen were determined. Correlation between rupture duration of the diaphragm and ignition delays are given. Comparison of experimental results with the previous numerical ones was carried out.

13/00913 Validation of a FLUENT CFD model for hydrogen distribution in a containment

Visser, D. C. *et al. Nuclear Engineering and Design*, 2012, 245, 161–171.

Hydrogen may be released into the containment atmosphere of a nuclear power plant during a severe accident. Locally, high hydrogen concentrations may be reached that can possibly cause fast deflagration or even detonation and put the integrity of the containment at risk. The distribution and mixing of hydrogen is, therefore, an important safety issue for nuclear power plants. Computational fluid dynamics (CFD) codes can be applied to predict the hydrogen distribution in the containment within the course of a hypothetical severe accident and get an estimate of the local hydrogen concentration in the various zones of the containment. In this way the risk associated with the hydrogen safety issue can be determined, and safety related measurements and procedures could be assessed. In order to further validate the CFD containment model of NRG in the context of hydrogen distribution in the containment of a nuclear power plant, the HM-2 test performed in the German THAI (thermal-hydraulics, hydrogen, aerosols and iodine) facility is selected. In the first phase of the HM-2 test a stratified hydrogen-rich light gas layer was established in the upper part of the THAI containment. In the second phase steam was injected at a lower position. This induced a rising plume that gradually dissolved the stratified hydrogen-rich layer from below. Phenomena that are expected in severe accidents, like natural convection, turbulent mixing, condensation, heat transfer and distribution in different compartments, are simulated in this hypothetical severe accident scenario. The hydrogen distribution and associated physical phenomena monitored during the HM-2 test are predicted well by the CFD containment model. Sensitivity analyses demonstrated that a mesh resolution of 45 mm in the bulk and 15 mm near the walls is sufficiently small to adequately model the hydrogen distribution and dissolution processes in the THAI HM-2 test. These analyses also showed that wall functions could be applied. Sensitivity analyses on the effect of the turbulence model and turbulence settings revealed that it is important to take the effect of buoyancy on the turbulent kinetic energy into account. When this effect of buoyancy is included, the results of the standard k–ε turbulence model and SST k–ω turbulence model are similar and agree well with experiment. The outcome of these sensitivity analyses can be used as input for setting up the guidelines on the application of CFD for containment issues.

13/00914 When solids meet solids: a glimpse into dust mixture explosions

Dufaud, O. *et al. Journal of Loss Prevention in the Process Industries*, 2012, 25, (5), 853–861.

Mixing an inert solid or a less flammable compound with a combustible dust can be regarded as a direct application of the inherent safety principle of moderation. An experimental investigation was carried out to determine the evolution of the ignition sensitivity and the explosion severity of such various mixtures as a function of their compositions. It demonstrates that the introduction of small amounts of highly combustible powders (such as sulfur or nicotinic acid) to a less flammable dust (such as microcrystalline cellulose or carbon black) can strongly influence the ignition sensitivity as well as the explosion severity. It has notably been shown that the ignition sensitivity of solid/solid mixtures significantly rises up when only 10–5 wt% of highly flammable dust is introduced. Simple models can often be applied to estimate the minimum ignition energy, minimum ignition temperature and minimum explosive concentration of such mixtures. Concerning the dust explosivity, three cases have been studied: mixtures of combustibles dusts without reaction, dusts with reactions between the powders, combustible dusts with inert solid. If the evolution of the maximum explosion pressure can be estimated by using thermodynamic calculations, the maximum rate of pressure rise is more difficult to predict with simple models, and both combustion kinetics and hydrodynamics of the dust clouds should be taken into account. These results were also extended to flammable dust/solid inertant mixture. They clearly show that the concentration of solid inertant at which the ignition is not observed anymore could reach 95 wt%. As a consequence, the common recommendation of solid inertant introduction up to 50–80 wt% to prevent dust explosion/ignition should be reconsidered.

09 PROCESS HEATING, POWER AND INCINERATION

Energy applications in industry

13/00915 A practical method for the maintainability assessment in industrial devices using indicators and specific attributes

De Leon, P. M. *et al. Reliability Engineering & System Safety*, 2012, 100, 84–92.

The objective of this paper is to describe a procedure to obtain maintainability indicators for industrial devices. This analysis can be helpful, among other cases, to compare systems, to achieve a better design regarding maintainability requirements, to improve this maintainability under specific industrial environment and to foresee maintainability problems due to eventual changes in a device operation conditions. This maintainability assessment can be carried out at any stage of the industrial asset life cycle. With this purpose, this work first introduces the notion of maintainability and the implementation of assessment indicators, including some important requirements to perform that. Then, a brief literature review is presented, including the definition of the main concepts, which are later used in the paper. After studying the maintenance levels and the maintainability attributes, both terms are linked, leading all this analysis to the assessment of the maintainability indicators. It follows a discussion about the information obtained through the maintainability assessment process and its computation into several maintainability indicators. The paper includes a case study, which implements the defined assessment into a practical scenario. Finally, the work concludes summarizing the more significant aspects and suggesting future researches.

13/00916 A rapid and low energy consumption method to decolorize the high concentration triphenylmethane dye wastewater: operational parameters optimization for the ultrasonic-assisted ozone oxidation process

Zhou, X. J. *et al. Bioresource Technology*, 2012, 105, 40–47.

This research set up an ultrasonic-assisted ozone oxidation process (UAOOP) to decolorize the triphenylmethane dyes wastewater. Five factors – temperature, initial pH, reaction time, ultrasonic power (low frequency 20 kHz), and ozone concentration – were investigated. Response surface methodology was used to find out the major factors influencing color removal rate and the interactions between these factors, and optimized the operating parameters as well. Under the experimental conditions: reaction temperature 39.81 °C, initial pH 5.29, ultrasonic power 60 W and ozone concentration 0.17 g/L, the highest colour removals were achieved with 10 min reaction time and the initial concentration of the MG solution was 1000 mg/L. The optimal results indicated that the UAOOP was a rapid, efficient and low energy consumption technique to decolorize the high concentration MG wastewater. The predicted model was approximately in accordance with the experimental cases with correlation coefficients R^2 and R^2_{adj} of 0.9103 and 0.8386.

13/00917 A systematic framework for the feasibility and technical evaluation of reactive distillation processes

Shah, M. *et al. Chemical Engineering and Processing: Process Intensification*, 2012, 60, 55–64.

This study presents a novel design methodology for the feasibility and technical evaluation of reactive distillation (RD), and discusses the applicability of various design methods of RD. The proposed framework for the feasibility evaluation determines the boundary conditions (e.g. relative volatilities, target purities, equilibrium conversion and equipment restriction), checks the integrated process constraints, evaluates the feasibility and provides guidelines to any potential RD process application. Providing that a RD process is indeed feasible, a technical evaluation is performed afterward in order to determine the technical feasibility, the process limitations, working regime and requirements for internals as well as the models needed for RD. This approach is based on dimensionless numbers such as Damkohler and Hatta numbers, as well as the kinetic, thermodynamic and mass transfer limits. The proposed framework for feasibility and technical evaluation of reactive distillation allows a quick and easy feasibility analysis for a wide range of chemical processes. In this work, several industrial relevant case studies – for example, synthesis of di-methyl carbonate (DMC), methyl acetate hydrolysis, toluene hydrodealkylation (HDA) process, fatty acid methyl esters (FAME) process and unsaturated polyesters synthesis – clearly illustrate the validity of the proposed framework.

13/00918 Assessment model for equipment risk management: petrochemical industry cases

Huang, R.-H. *et al. Safety Science*, 2012, 50, (4), 1056–1066.

This study presents an assessment model that examines quantity and quality factors for equipment risk management in the petrochemical industry. The proposed model has five dimensions: financial performance, logistical support, service level, learning and innovation, and risk control. This evaluation model uses 13 strategy subjects and 78 performance-measurement indicators. Performance assessment indicators are initially established and revised based on expert opinions collected via a questionnaire. Further, the analytical network process (ANP) is utilized to calculate the weights of indicators in each layer and to construct assessment models with applicable and valuable references. To determine model practicability, this study assesses four subsidiaries of the case company. Each subsidiary has a capitalization exceeding TWD50 billion. In addition to evaluating company performance in terms of each dimension and indicator, the proposed model provides a valuable reference for decision-making in equipment risk management.

13/00919 Carbon nanotube/carbon nanofiber growth from industrial by-product gases on low- and high-alloy steels

Gaikwad, A. V. *et al. Carbon*, 2012, 50, (12), 4722–4731.

The growth of carbon nanotubes (CNTs) on sheet metal surfaces (including low- and high-alloyed steel and Ni-plated steel) has been explored using a mixture of CO, CO_2, and H_2 as the precursor feedstock in a thermal chemical vapour deposition process. The influence of various experimental parameters such as the reactor temperature, reaction time, and precursor composition on the yield, purity, and dimensions of the CNTs has been elucidated. Addition of CO_2 during CNT growth leads to higher carbon deposition rates, especially for low- and high-alloyed steel. The diameters of the obtained CNTs range from 12 to 300 nm at carbon deposition rates of $\sim 0.3\,\mathrm{mg\,cm^{-2}\,min^{-1}}$. The CNTs are observed to be uniformly distributed and adhered firmly to the substrates. The experimental conditions for CNT growth on sheet metal surfaces are very similar to concentrations and temperatures of a typical effluent stream of the steel industry. This process thus holds potential to harness waste gases to fabricate CNT-based coatings that impart added functionality to sheet metals, while further reducing the carbon footprint of steel plants.

13/00920 Comparative analysis of low temperature industrial refrigeration systems

Mumanachit, P. *et al. International Journal of Refrigeration*, 2012, 35, (4), 1208–1221.

This paper compares the energy performance and economics of a direct two-stage ammonia system to an ammonia–carbon dioxide cascade system for low temperature (below −40 °C) applications. Component and system models are developed for both the direct ammonia and the ammonia–carbon dioxide cascade options. These models provide the basis for quantifying the relative operating costs for both systems on annual and life-cycle bases. The analysis shows that the ammonia–carbon dioxide cascade system option using a shell-and-tube cascade condenser offers the potential for increased energy efficiency when compared to a direct two-stage ammonia system when operating with evaporating temperatures that are below −46.2 °C. For the cascade system option, the analysis shows that a shell-and-tube cascade heat exchanger with design approach temperature of 5.6 °C provides the optimal balance of system performance with capital cost.

13/00921 Convective cooling optimization of a blade for a supercritical steam turbine

Nowak, G. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4511–4520.

This paper discusses the problem of blade cooling system optimization connected with conjugate heat transfer (CHT) analysis for reliable thermal field prediction within a steam cooled component. Since the full CHT solution, which involves the main flow, blade material and the coolant flow domains is computationally expensive from the point of view of optimization process, it was decided to reduce the problem by fixing the boundary conditions at the blade surface and solving the task for the interior only (both solid material and coolant). Such assumption, on one hand, makes the problem computationally feasible, and on the other, provides more reliable thermal field prediction than it used to be with the empirical relationships. The analysis involves shape optimization of internal cooling passages within an airfoil. The cooling passages are modelled with a set of four Bezier splines joined together to compose a closed contour. Each passage is fed with cooling steam of constant parameters at the inlet. In the present study the airfoil profile is taken as aerodynamically optimal. The search problem is solved with evolutionary algorithm and the final configuration is to be found among the Pareto optimal cooling candidates.

13/00922 Eco-innovative design method for process engineering

Ferrer, J. B. *et al. Computers & Chemical Engineering*, 2012, 45, 137–151.

Due to the environmental issues, innovation is one way to challenge eco-friendly technologies, create new process options which are needed to meet the increasing demands for sustainable production. To accelerate and improve eco-innovative design, there is a need for the computer aided eco-innovation tools to support engineers in the preliminary design phase. Currently, several computer aided innovation tools with a clear focus on specific innovation tasks exist but very few of them deal with the eco-innovation issues. Therefore the purpose of this paper is to present the development of a computer aided model based preliminary design methodology focused on technological eco-innovation for chemical engineering. This methodology is based on modified tools of the structured TRIZ theory. The general systematic framework gives the same level of importance, to the technological and environmental requirements during the conceptual design phase. Integrating environment oriented design approach at the earliest, in the design phase, is essential for product effectiveness and future development. The methodology employs a decomposition based solution approach in hierarchical steps by analysing the problem faced, formulation of the problem and the generation of possible and feasible ideas. At each step, various methods and tools will be needed. In this paper some existing tools are adapted to chemical engineering and some tools of the structured TRIZ theory are modified and improved to build a specific methodology oriented towards the increasing technological complexity and environmental issues of current designs. Undoubtedly, the selection of materials and substances for a particular generated concept, mainly affects the structure, mechanical factors (processability and dimensions) and the environmental impact. In order to deal with these environmental criteria, the resources and their impacts are considered in the upstream phase of the design process and are introduced as constraints in the model. To highlight its capabilities, the methodology is illustrated through a case study dedicated to tars and ashes issues in biomass gasification.

13/00923 From ammonium bicarbonate fertilizer production process to power plant CO_2 capture

Zhuang, Q. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 56–63.

Ammonia-based CO_2 capture technology has attracted wide research interest. Substantial work has been reported that includes theoretical evaluation, laboratory tests, pilot plant tests and economic analysis. Alstom and PowerSpan have conducted a few MW level demonstration tests. However, three inherent hurdles with this potential CO_2 capture technology have not been fully solved yet: ammonium bicarbonate solid formation in the absorption tower which may plug the tower packing, high ammonia vapour pressure that results in ammonia slip into the cleaned flue gas, and low CO_2 absorption rate resulting in large absorption equipment. Industrial ammonium bicarbonate fertilizer production processes are proven technology and have been optimized both technologically and economically for decades. This technology is also based on the chemistry and physics of the NH_3–CO_2–H_2O system. In the ammonia synthesis plant, CO_2 in shifted gas from the syngas obtained by gasification of coal is absorbed into partly carbonated aqueous ammonia in a liquid bubbling column to produce ammonium bicarbonate solid as fertilizer. Using this process, ammonium bicarbonate has been sustainably produced with low ammonia slip into the shifted gas after the CO_2 was captured. In this report, the ammonium bicarbonate fertilizer production process is described and analysed. The advantageous aspects of the fertilizer production technology are compared with the current widely studied ammonia-based CO_2 capture technology for power plant applications. Insights into the modifications required for the flue gas CO_2 capture application are discussed. New designs of ammonia-based CO_2 capture processes are presented.

13/00924 Heat transfer characteristics of natural gas/air swirling flame impinging on a flat surface

Singh, G. *et al. Experimental Thermal and Fluid Science*, 2012, 41, 165–176.

An experimental study has been conducted to investigate the heat transfer characteristics of compressed natural gas (CNG)/air swirling flames impinging on a flat surface. Qualitative flame structures have been studied by taking direct photographs of impinging flames. The radial temperature distribution of swirling free and impinging flames is presented at different axial heights under fixed operating conditions. Effects of dimensionless separation distance (1–6), Reynolds number (3500–6000), equivalence ratio (1–1.5) and helical vane swirler angle (0–60°) on heat transfer characteristics have been investigated. The heat transfer characteristics of swirling and non-swirling flames have been compared under similar operating conditions. A dip in the heat flux at and around stagnation point was observed in almost all cases which could be the main cause of non-uniformity even in case of heating with swirling impinging flames. The dip in heat flux becomes more pronounced at higher Reynolds number. The heat flux distribution on the impingement plate was more uniform with swirl as compared to without swirl. Also, heat flux distribution was observed to be more uniform at moderate separation distance and at larger helical vane swirl angle. Stagnation point heat flux variation remains almost constant at higher separation distances for different values of Reynolds number and equivalence ratios. There was significant decrease in average heat flux with increase in separation distance. It was further observed that average heat flux increases sharply with Reynolds number whereas the variation was not that steep with change in equivalence ratio.

13/00925 Kletz's legacy for developing countries: simple systems based on inherently safer design

Gómez, G. *et al. Journal of Loss Prevention in the Process Industries*, 2012, 25, (5), 843–847.

The now well-known theory surrounding inherently safer design (ISD) has spread worldwide. This means that developing countries, such as Colombia, now have the possibility of applying it to their specific situations, which can often be resolved if the safety hierarchy is followed in order to attack problems from the design stage, a solution that might not seem instinctive, but is actually effective since there is no 'reduction' strategy, but a removal of hazards. To apply this methodology to a specific Colombian case study, a previous quantitative risk analysis of a liquefied petroleum gas (LPG) storage tank farm in Colombia is revised and reformulated by developing an optimization (MINLP) based on the principles of inherent safety in order to design the same process (LPG pressurized storage) so that the available engineering tools can be used to mathematically formulate the inherent safety criteria. This allows determining the design conditions and safety measures needed to reduce the likelihood of an incident, being consistent with the inherent safety philosophy, which seeks a change of mental structure when designing processes. The results of the project allow obtaining a specific optimal configuration of control, wall thickness, operating pressure and tank dimensions, pointing out a decrease of around 20% on the operating pressure.

13/00926 Mercury stable isotope fractionation in six utility boilers of two large coal-fired power plants

Sun, R. *et al. Chemical Geology*, 2012, 336, 103–111.

Coal-fired utility boiler (CFUB) emissions of mercury (Hg) represent the largest anthropogenic Hg source to the atmosphere. Hg stable isotope signatures in coal have been shown to vary among coal deposits and coal basins. There is therefore a substantial interest in tracing CFUB Hg emissions at local, regional and global scales. However, CFUB operating conditions, Hg capture technologies and post-emission Hg transformations may potentially alter the original feed coal Hg isotope signatures. Here the authors investigate Hg isotopic fractionation between feed coal and coal combustion products in six utility boilers of two large power plants in Huainan City, Anhui Province, China. They observed identical trends in all six boilers: relative to feed coal with δ^{202}Hg ranging from −0.67 to −0.18‰, oxidized Hg species in bottom ash and fly ash are enriched in the lighter isotopes with δ^{202}Hg from −1.96 to −0.82‰. Flue gas desulfurization by-product gypsum shows δ^{202}Hg from −0.99 to −0.47‰. No mass independent fractionation was observed during the transport and transformation of Hg inside the boilers. An isotope mass balance suggests that gaseous stack Hg emissions are enriched by up to 0.3‰ in the heavier Hg isotopes relative to feed coal and that the enrichment depends on the Hg capture technology. The observation that oxidized Hg species are enriched in the lighter isotopes suggests that oxidized and reduced forms of Hg in stack emission carry different isotope signatures. This has implications for near-field and far-field Hg emission tracing.

13/00927 Numerical simulation and theoretical study on simultaneously effects of operating parameters in direct contact membrane distillation

Bahmanyar, A. *et al. Chemical Engineering and Processing: Process Intensification*, 2012, 61, 42–50.

Effect of operating conditions such as feed temperature, feed circulation rate and feed inlet concentration on permeate flux in a direct contact membrane distillation (DCMD) have been simulated. The effects of these parameters on both temperature and concentration polarizations have also been taken into account. A simultaneous heat and mass transfer model has been used in the DCMD system. The model has been solved numerically using MATLAB. Significances of the heat transfer due to mass flux, heat lost by conduction, as well as their contribution to the overall heat flux through the membrane have been determined. The variation of physical and flow properties with temperature and consequently heat transfer coefficients have been considered in this study. The influence of mass transfer on heat transfer coefficients and heat transfer rates has been considered in heat transfer equations. Finally, the simultaneously effects of the operating parameters on response variables have been studied.

13/00928 Optimal reconfiguration of multi-plant water networks into an eco-industrial park

Rubio-Castro, E. *et al. Computers & Chemical Engineering*, 2012, 44, 58–83.

This paper presents an MINLP model to design an eco-industrial plant by retrofitting existing water networks from different industrial plants in the same industrial zone. The proposed model is based on a superstructure and takes into account both in-plant and inter-plant structural modifications, such as the placement/reassignment of existing treatment units, the required increase of capacity and/or efficiency of existing treatment units, the placement of new treatment units either within the participating plants or in a new shared wastewater treatment facility, and the stream re-piping associated with installing new treatment units and retrofitting existing treatment units. The model allows the tracking of changes in the process performance as a result of the stream re-routing and retrofitting activities. Two examples were solved, and the results show the economic and environmental benefits of the retrofitted networks within an eco-industrial park compared to the stand-alone retrofitted networks.

13/00929 Process integration of steelmaking and methanol production for suppressing CO_2 emissions – a study of different auxiliary fuels

Ghanbari, H. *et al. Chemical Engineering and Processing: Process Intensification*, 2012, 61, 58–68.

In this work mathematical programing has been used to study the process economics, carbon dioxide emission and energy flows of a future steel plant which is integrated with a polygeneration plant. The system considered includes an integrated steelmaking plant with conventional or novel ironmaking technologies with top gas recycling and CO_2 stripping, a CHP plant and a methanol plant. Oil, natural gas and biomass are considered as both auxiliary reducing agents in the blast furnace and also as fuel in the polygeneration system. The results illustrate that an integration of steelmaking with a polygeneration system will increase the total energy efficiency and decrease the emissions of the system. It is demonstrated that certain combination of new technologies and alternative fuels yield scenarios with strongly reduced emissions, indicating a path to sustainable development in steelmaking.

13/00930 Process plant safety information repository and support for safety applications

Chung, P. W. H. *et al. Journal of Loss Prevention in the Process Industries*, 2012, 25, (5), 788–796.

The consideration of safety of processing plants from design to operation involves many tasks. Different techniques and tools have been developed to assist in carry out those tasks. With the advances in computing technologies, both in hardware and software, there is the opportunity to bring together the vast amount of engineering, hazard and risk data and handle them in an efficient way to manage and improve safety throughout the life time of a plant. This paper proposes keeping such data in a process plant safety information repository which can be easily accessed by different safety-related tools to enhance the efficiency of safety identification and analysis tasks.

13/00931 Recovering wastes from the paper industry: development of ceramic materials

Martínez, C. *et al. Fuel Processing Technology*, 2012, 103, 117–124.

The continuous generation of industrial waste and the environmental problems it causes make it necessary to seek alternative methods for treating waste. The development of ceramic materials seems to be one such alternative. This paper considers the possibility of recovering two forms of waste from the paper industry, sludge from the purification of waste water and residue from cleaning the pulp. The sludge and residue can be used in ceramics, whose properties and composition permit the incorporation of such waste in their manufacture. This addition enables savings in both raw materials and energy, as these waste products have high calorific content. In both cases, the results show that increasing the content of waste increases linear expansion and water absorption and in turn reduces resistance to compression. The decrease in resistance to compression is more pronounced in the specimens prepared with paper waste than in those prepared with sludge. The results also show a decrease in thermal conductivity that is attributable to the lightening quality of both residues.

13/00932 Review of technologies for mercury removal from flue gas from cement production processes

Zheng, Y. *et al. Progress in Energy and Combustion Science*, 2012, 38, (5), 599–629.

Mercury is a pollutant of concern and mercury emissions from cement plants are under environmental regulation. After coal-fired power plants, mercury emissions from cement and mineral production are the second largest anthropogenic sources. Compared to fuels, cement raw materials are the major sources of mercury in the cement kiln flue gas. Cement plants are quite different from power plants and waste incinerators regarding the flue gas composition, temperature, residence time, and material circulation. Cement kiln systems have some inherent ability to retain mercury in the solid materials due to the adsorption of mercury on the solids in the cold zone. However, recirculation of the kiln dust to the kiln will cause release of the captured mercury. The mercury chemistry in cement kiln systems is complicated and knowledge obtained from power plants and incinerators cannot be directly applied in cement kilns. Among the mercury control technologies, sorbent injection upstream of a particulate control device has shown the most promise. Due to material recirculation, and high moisture level in the cement kiln flue gas the application of sorbent injection to cement plants will be more challenging. The sorbent injection system should be installed downstream of the main kiln filter and upstream of a new added polishing fabric filter to avoid the cement kiln dust recycling and disposal issues. To reduce the sorbent cost and possible disposal expense, non-carbon-based sorbents that could be added to cement or regenerated *in situ* are desired and should be developed. Various mathematical models have been developed to simulate mercury removal in fixed-bed reactors and by sorbent injection upstream of a fabric filter. The fabric filter adsorption models use the adsorption isotherms coupled with diffusion in the sorbent particle and the parameters are obtained by fitting the model to experimental data. Verification of the models by full-scale or pilot-scale data is very limited.

13/00933 Simulation of industrial-scale CO_2 storage: multi-scale heterogeneity and its impacts on storage capacity, injectivity and leakage

Deng, H. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 397–418.

Heterogeneities in porosity and permeability of geological CO_2 storage reservoirs and surrounding strata have a significant influence on storage capacity, design of injection wells, CO_2 injection rate, potential leakage, CO_2 plume migration, and risk assessment. This study develops a methodology that applies a transition probability based Markov chain model to generate facies-based heterogeneous fields of reservoir and cap-rock porosity and permeability at the Rock Springs Uplift, Wyoming. This site was chosen for its proximity to the Jim Bridger power plant that generates 18 Mt of CO_2 per year. The heterogeneous fields are then used as input to simulations of CO_2 injection in a numerical domain with geologic strata based on a three-dimensional seismic model. The authors next use the multiphase flow simulator FEHM in Monte Carlo mode to generate 42 realizations of injection into the Weber sandstone. The model is constrained by two requirements. First, the effects of storage must be contained in the 16 × 16 km working footprint (i.e. the injection pressure pulse and CO_2 plume are not allowed to expand beyond the simulation domain) and second, injection pressures must not exceed 75% of the lithostatic load to limit seismic risks. Analysis of simulation results reveals that: (1) CO_2 storage capacity for the Weber formation in the entire Rock Springs Uplift is 6614 ± 256 Mt at 95% confidence interval, about 36% of a previous estimate based on homogeneous and isotropic properties; (2) single well CO_2 injection rates vary with time and with local permeability distributions. The injectivity at the end of 50 years of injection follows a log normal distribution and reaches a mean of 0.43 Mt/year with a range of 0.06–3.22 Mt/year within two standard deviations ($1\sigma = 0.09$ Mt/year); and (3) CO_2 leakage into the cap-rock (Chugwater formation) is limited to 0.8 ± 3. Mt over the 50 years of injection. In addition, brine production rates required to maintain pressure in the working footprint are of nearly equal volume to the injected CO_2. Within the CO_2 plume at this deep site, CO_2 has density of greater than 80% of the ambient brine, indicating that the CO_2 plume evolution will be controlled more by fluid pressure gradients than by buoyant flow. These results suggest that injection into the Weber sandstone in a single 16 × 16 km working footprint on the Rock Springs Uplift could likely store the total CO_2 output of the Jim Bridger power plant for approximately 35 years with less than 1% leakage into the cap-rock. This plan would require 26 ± 3 injection wells with likely an equal number or more of brine production wells around the perimeter of the working footprint. Assuming wells at a cost of $6 million each, this would add less than $1/tonne to the cost of the storage, a small fraction of current capture costs. Finally, brine production on the order of 1 km^3 is required to minimize the risk of geomechanical failure and ensure limited pressure perturbation outside the working footprint.

13/00934 Sliding mode control (SMC) of permanent magnet synchronous generators (PMSG)

Merzoug, M. S. *et al. Energy Procedia*, 2012, 18, 43–52.

This paper presents sliding mode control of permanent magnet synchronous generators (PMSG). A comprehensive dynamical model of the PMSG in *d–q* frame and its control scheme is presented. Wind energy is a promising technology and becomes a more and more interesting player on the market of energy production. Since the converter/capacitor model is non-linear, the sliding mode technique constitutes a powerful tool to ensure the dc-bus voltage regulation. The simulation results show the method is simple and has high precision of control, and the system has good characteristics in steady state and during transients with permanent magnet synchronous generator.

13/00935 Steps towards sustainable manufacturing through modelling material, energy and waste flows

Smith, L. and Ball, P. *International Journal of Production Economics*, 2012, 140, (1), 227–238.

A sustainable society cannot be realized without more efficient approaches and technologies, which must in part be provided by manufacturing. Available literature covers the principles for making manufacturing more sustainable, but there is little, if any, practical guidance to show how to apply these principles. Lower level guidelines are required to provide guidance on systematically analysing manufacturing facilities and to assist with the identification and selection of improvement opportunities. This paper reports on work to develop guidelines for material, energy and waste (MEW) process flow modelling to support the pursuit of sustainable manufacturing. Using qualitative MEW process flow maps of a case facility, data was collected to build a spreadsheet model aligned to each of the MEW process flows. The quantitative analysis provided detailed insight into the MEW process flows within the system and assisted with the identification and selection of environmental efficiency improvements. The key learning points from conducting the analysis generated a set of guidelines to aid the analysis of manufacturing systems, using MEW process flow modelling. This paper documents the approach developed and the environmental performance improvement opportunities identified in the case facility.

13/00936 The carbon footprint and energy consumption of a commercially produced earthenware ceramic piece

Quinteiro, P. *et al. Journal of the European Ceramic Society*, 2012, 32, (10), 2087–2094.

The product carbon footprint quantifies the greenhouse gas (GHG) emissions during the life cycle of a product, from the extraction of raw materials, through the production, use and recycling, to the disposal of the used product. In this study, the carbon footprint of an ornamental earthenware ceramic piece has been estimated following the PAS 2050:2011 methodology, and the energy and GHG hotspots have been identified. The carbon footprint and the total energy consumption of the selected ceramic piece is 1.22 kg CO_2e per piece and 8.19 kWh, respectively. The manufacture represents almost 90% of the carbon footprint of the piece. The energy hotspots are natural gas production, biscuit firing and condensing boiler. Some measures to reduce the consumption of natural gas and electricity have been applied, such as the implementation of a gas pressure control system in the kilns and the mill lighting system optimization, respectively.

13/00937 The feasibility of the sustainable energy supply from bio wastes for a small scale brewery – a case study

Sturm, B. *et al. Applied Thermal Engineering*, 2012, 39, 45–52.

In the food industry, a significant percentage of raw materials used leaves the process as biological waste. In this study a small-scale brewery situated in north-east England was audited. Based on the data obtained, the feasibility of biogas generation was modelled. The model included a planned extension to production capacity. Several scenarios for conversion were simulated, their gas demand determined, performance compared and economic viability calculated. The use of production waste along with manure from nearby farms proved to be suitable to provide the amount of fuel needed for all scenarios investigated. The integration of an anaerobic digester plant on the premises of the brewery investigated would be very easy to realize as it is situated on a former farm with its own well. As process temperatures are comparatively low, a steam boiler as well as a combined heat and power (CHP) system could be used to provide for the heat needed. The use of the CHP would allow for simultaneous generation of heat and electricity required as well as a potential to export excess electricity to the national grid. Both solutions qualify for the governmental funding schemes both the thermal as well as the electrical energy demand are below the maximum limit for funding. Implementation of a trigeneration system is not feasible as refrigeration is needed constantly on a very low power level while heat is only needed during production. Opposed to that running an absorption chiller on the biogas produced is a solution to be considered as it qualifies for the renewable heat incentive. The combination of either, boiler or CHP with an absorption chiller are considered the most viable solutions as they create the shortest payback periods and higher additional income than the solutions without. As the former solution is more than £200,000 cheaper than the latter and the integration in the existing system would be easier this could be the preferable solution for a small company although this also means a reduction of additional income by roughly 30% from £1884 to £1310. The application of biogas has an effect of net zero carbon emission, and is potentially, making the enterprise more sustainable in future as well as creating an additional saving potential regarding carbon trading. Due to growing issues with complaints about odour nuisance when applying slurry directly on the field an additional advantage of co-digesting brewer's waste and cattle manure is the production of highly valuable fertilizer that is free of smell.

13/00938 The hydrogen adsorption capacity of commercial Pd/Rh and Pt/Rh automotive catalysts and its relationship to their activity

Fernandes, D. M. *et al. Chemical Engineering Journal*, 2012, 189–190, 62–67.

Recent papers studying both fresh and aged Pt–Rh and Pd–Rh commercial catalysts reported hydrogen programmed temperature desorption (H_2-TPD) results in an attempt to determine the noble metal dispersion. However, for the fresh catalysts, the total amount of adsorbed H_2 was greater than the quantity of noble metals determined via chemical analysis, which indicates other processes, such as hydrogen spillover and H_2 interactions with the ceria support, can contribute to the hydrogen adsorption. These results have now been reviewed, and although they cannot be used to determine the metal dispersion, a correlation between them and the catalytic activities for both propane and CO oxidation and the reduction of NO by CO was found. As catalytic activities are influenced by nearly all of the washcoat components, such as ceria–zirconia mixed oxides and nickel oxide, in addition to the noble metals, in some way, this technique appears to dose the sites (metal and support) involved in the catalytic reaction. Therefore, H_2-TPD can be used for comparison of the catalytic activity of these catalysts.

13/00939 Thermohydraulics of laminar flow of viscous oil through a circular tube having integral axial rib roughness and fitted with center-cleared twisted-tape

Saha, S. K. *et al. Experimental Thermal and Fluid Science*, 2012, 41, 121–129.

The experimental friction factor and Nusselt number data for laminar flow through a circular duct having integral axial rib roughness and fitted with centre-cleared twisted-tape have been presented. Predictive friction factor and Nusselt number correlations have also been presented. The thermohydraulic performance has been evaluated. The major findings of this experimental investigation are that with and without centre-cleared twisted tapes in combination with integral axial rib roughness perform significantly better than the individual enhancement technique acting alone for laminar flow through a circular duct up to a certain amount of twisted-tape centre-clearance.

13/00940 Two phase steady-state particle size distribution in a gas-phase fluidized bed ethylene polymerization reactor

Ashrafi, O. *et al. Chemical Engineering Science*, 2012, 73, 1–7.

A population balance model is developed to investigate the steady state particle size distribution developments in a gas-phase fluidized-bed ethylene polymerization reactor. The model considers the combined effects of particle growth and elutriation for size distributed prepolymer feed. In the proposed model, the bed is divided into several sections consisting of bubble and emulsion phases. The population balance differential equations derived for each section were simultaneously solved to determine the density function of the size distribution of the polymer particles in each section. The model is able to estimate the axial profile of particle size distribution along the reactor height. It was shown that the mean size of the particles is larger at the bottom of the bed and becomes smaller when moving toward top of the reactor. The size distribution of the polymer particles in the product becomes sharper and their mean size decreases by increasing the superficial gas velocity. Also, mean size of the particles in the product increases by increasing the temperature of the reactor.

13/00941 Using modified Barabási and Albert model to study the complex logistic network in eco-industrial systems

Xiao, Z. *et al. International Journal of Production Economics*, 2012, 140, (1), 295–304.

In recent years, both researchers and practitioners have devoted attention to environmental sustainability issues in the green supply industry, but, how to design the green logistic network in the eco-industrial system is missing. This article reports on the study of designing green logistic network in an eco-industrial system by modifying the Barabási and Albert (BA) model based on the intrinsic properties of eco-industrial systems. After verifying that the modified BA model is more accurately to interpret the formation mechanism of an eco-industrial network by the mean-field approach, paper extended and generalized some basic rules of the In-degree and Out-degree distributions of an EIN under the influences of different factors to assist eco-manufactures choose their supplier or customer, even design their own supplying networks by application of complex networks theory with the aid of the Jinjie EIS case example.

10 SPACE HEATING AND COOLING/HEAT PUMPS

13/00942 A bimetallic micro heat engine for pyroelectric energy conversion

Thundiparambu Ravindran, S. K. *et al. Procedia Engineering*, 2012, 47, 33–36.

The authors present a novel concept of electric power generation from a spatial temperature gradient, achieved by integrating pyroelectric generators (PEGs) into a self-oscillating micro heat engine. The micro heat engine moves the PEGs between a hot and cold reservoir, thus bringing them in an alternating contact with a higher and lower temperature. By their pyroelectric nature, the PEGs convert this periodic temperature variation into electrical energy. The micro heat engine is fabricated from a 280 μm thick bimetallic strip and the PEGs from a 250 μm thick PZT sheet. At an oscillation frequency of 0.19 Hz the device generates 4.4 μW of electrical power from a 96 K temperature difference.

13/00943 A combined experimental and computational study on the melting behavior of a medium temperature phase change storage material inside shell and tube heat exchanger

Hosseini, M. J. *et al. International Communications in Heat and Mass Transfer*, 2012, 39, (9), 1416–1424.

A combined experimental and numerical study is performed aiming to understand the role of buoyancy-driven convection during constrained melting of phase change materials (PCMs) inside a shell and tube heat exchanger. A series of experiments is conducted to investigate the effect of increasing the inlet temperature of the heat transfer fluid (HTF) on the charging process (melting) of the PCM. The computations are based on an iterative, finite-volume numerical procedure that incorporates a single-domain enthalpy formulation for simulation of the phase change phenomenon. It was observed from experimental results that the melting front appeared at different times at positions close to the HTF tube and progressing at different rates outwards towards the shell. The computational results show that by increasing the inlet water temperature to 80 °C, the total melting time is decreased to 37%.

13/00944 A lattice Boltzmann method for simulation of liquid–vapor phase-change heat transfer

Gong, S. and Cheng, P. *International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4923–4927.

A lattice Boltzmann model for the liquid–vapour phase change heat transfer is proposed in this paper. Two particle distribution functions, namely the density distribution function and the temperature distribution function, are used in this model. A new form of the source term in the energy equation is derived and the modified pseudo-potential model is used in the proposed model to improve its numerical stability.

The commonly used Peng–Robinson equation of state is incorporated into the proposed model. The problem of bubble growth and departure from a horizontal surface is solved numerically based on the proposed model.

13/00945 A reduced-order model for heat transfer in multiphase flow and practical aspects of the proper orthogonal decomposition

Brenner, T. A. *et al. Computers & Chemical Engineering*, 2012, 43, 68–80.

This paper discusses two practical aspects of reduced-order models (ROMs) based on proper orthogonal decomposition (POD) and presents the derivation and implementation of a ROM for non-isothermal multiphase flow. The POD method calculates basis functions for a reduced-order representation of two-phase flow by calculating the eigenvectors of an autocorrelation matrix composed of snapshots of the flow. The flow is divided into transient and quasi-steady regions and two methods are shown for clustering snapshots in the transient region. Both methods reduce error as compared to the constant sampling case. The ROM for non-isothermal flow was developed using numerical results from a full-order computational fluid dynamics model for a two-dimensional non-isothermal fluidized bed. Excellent agreement is shown between the reduced- and full-order models. The composition of the autocorrelation matrix is also considered for an isothermal case. An approach treating field variables separately is shown to produce less error than a coupled approach.

13/00946 AC voltage induced electrohydrodynamic two-phase convective boiling heat transfer in horizontal annular channels

Cotton, J. S. *et al. Experimental Thermal and Fluid Science*, 2012, 41, 31–42.

An experimental study of alternating current (AC) induced electrohydrodynamic (EHD) flow and heat transfer augmentation for boiling inside an annular channel containing working fluid refrigerant HFC-134a has been conducted in a single-pass, counter-flow heat exchanger with a rod electrode placed concentric to a grounded tube. Experiments were conducted for an inlet quality of 0%, a heat flux of 10.2 kW/m^2, mass fluxes from 100 kg/m^{2}s to 500 kg/m^{2}s and applied voltages from 0 to 8 kV DC and 0 to 24 kV peak to peak AC. The AC tests were conducted for both low frequency (60 Hz) and high frequency (6.6 kHz) near sinusoidal waveforms. The results show that there is no apparent difference between the DC and the 6.6 kHz AC test cases, whereas the 60 Hz AC tests show significantly different behaviour. The flow boiling heat transfer results indicate that the averaged heat transfer coefficients can be increased by as much as three-fold for a 24 kV peak to peak 60 Hz AC applied voltage. This also incurs a pressure drop penalty of 2.6-fold across the heat exchanger.

13/00947 An experimental investigation of enhanced thermal conductivity and expedited unidirectional freezing of cyclohexane-based nanoparticle suspensions utilized as nano-enhanced phase change materials (NePCM)

Fan, L. and Khodadadi, J. M. *International Journal of Thermal Sciences*, 2012, 62, 120–126.

An experimental investigation of nanoparticle suspensions utilized as nano-enhanced phase change materials (NePCM) was conducted. Cyclohexane-based NePCM samples were prepared with copper oxide nanoparticles with various mass concentrations. Thermal conductivity of the samples was measured using the transient plane source technique for both liquid and solid phases at multiple temperatures. Unidirectional freezing of the samples was investigated and the experimental results were compared with the numerical predictions of a one-dimensional Stefan model proposed earlier by the authors. It was shown that the measured thermal conductivity for samples in their liquid phase is enhanced with increasing concentration of nanoparticles, whereas the data in the solid phase exhibit a non-monotonic enhancement when the concentration is greater than 2%. Unidirectional freezing was found to be expedited by up to 5.2%.

13/00948 An experimental study on flow patterns and heat transfer characteristics during cryogenic chilldown in a vertical pipe

Hu, H. *et al. Cryogenics*, 2012, 52, (4–6), 268–277.

In the present paper, the experimental results of a cryogenic chilldown process are reported. The physical phenomena involve unsteady two-phase vapour–liquid flow and intense boiling heat transfer of the cryogenic fluid that is coupled with the transient heat conduction inside pipe walls. The objective for the present study is to compare the chilldown rates and flow patterns between the upward flow and downward flow in a vertical pipe. Liquid nitrogen is employed as the working fluid and the test section is a vertical straight segment of a Pyrex glass pipe with an inner diameter of 8 mm. The effects of mass flow rate on the flow patterns, heat transfer characteristics and interface movement were determined through experiments performed under several different mass flow rates. Through flow visualization, measurement and analysis on the flow patterns and temperature variations, a physical explanation of the vertical chilldown is given. By observing the process and analysing the results, it is concluded that pipe chilldown in a vertical flow is similar to that in microgravity to some extent.

13/00949 Analysis of a new cross flow heat exchanger flow arrangement – extension to several rows

Cabezas-Gómez, L. *et al. International Journal of Thermal Sciences*, 2012, 55, 122–132.

The present paper presents a theoretical analysis of a cross flow heat exchanger with a new flow arrangement comprehending several tube rows. The thermal performance of the proposed flow arrangement is compared with the thermal performance of a typical counter cross flow arrangement that is used in chemical, refrigeration, automotive and air conditioning industries. The thermal performance comparison has been performed in terms of the following parameters: heat exchanger effectiveness and efficiency, dimensionless entropy generation, entransy dissipation number, and dimensionless local temperature differences. It is also shown that the uniformity of the temperature difference field leads to a higher thermal performance of the heat exchanger. In the present case this is accomplished thorough a different organization of the in-tube fluid circuits in the heat exchanger. The relation between the recently introduced ‘entransy dissipation number’ and the conventional thermal effectiveness has been obtained in terms of the ‘number of transfer units’. A case study has been solved to quantitatively to obtain the temperature difference distribution over two rows units involving the proposed arrangement and the counter cross flow one. It has been shown that the proposed arrangement presents better thermal performance regardless the comparison parameter.

13/00950 Analysis of convective heat transfer at building façades in street canyons and its influence on the predictions of space cooling demand in buildings

Allegrini, J. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2012, 104–106, 464–473.

An important part of the world’s energy is used for space cooling of buildings. Minimization of space cooling, especially in hot urban environments, has great energy-saving potential. An important part of the heat exchange between buildings and the ambient surrounding is due to convective and radiative heat flows. The impact of these heat flows on energy consumption for cooling is much more important in urban areas compared to rural areas. This study aims at quantifying the influence of the urban radiation balance, the urban heat island effect and urban convective heat transfer coefficients (CHTC) on the space cooling demands. CHTC correlations were determined using computational fluid dynamics (CFD) for different geometries including stand-alone buildings and street canyons of different lengths. Buoyancy was accounted for by considering differences between building surface and surrounding air temperature. It was found that the building geometry has a large impact on the CHTC correlations and that the effect of buoyancy cannot be neglected when wind speeds are low. These CHTC correlations were used for building energy simulation (BES) predictions of the space cooling demand. Space cooling demands for a building in a street canyon differ up to a factor of 1.8 depending on the CHTC correlations used. Therefore, for accurate predictions of the space cooling demand, adequate CHTC correlations have to be used adjusted to the actual building configuration.

13/00951 Analysis of material effect in molten fuel–coolant interaction, comparison of thermodynamic calculations and experimental observations

Tyrpekl, V. and Piluso, P. *Annals of Nuclear Energy*, 2012, 46, 197–203.

Molten fuel–coolant interaction (FCI) is considered an important phenomenon in the frame of nuclear reactor severe accident research and development. Recently, the so-called ‘material effect’ in FCI was observed in several experimental research programs. It was found that chemically different melts yield to different explosion energetics or trigger-ability during FCI tests. The presented work is focused on the thermodynamic modelling of high temperature chemical reactions during the melt–coolant interaction and consequent comparison with results obtained by material analyses of debris coming from KROTOS (CEA, France), MISTEE (KTH, Sweden) and PREMIX (FZK, Germany) experimental research programs. Calculations at thermodynamic equilibrium were obtained using the Gemini 2 (Thermodata) Gibbs energy minimizer. Information about debris composition, morphology and structure were collected using solid-state characterization techniques such as scanning electron microscopy, X-ray powder diffraction and thermogravimetry. Chemical reactions of melt and water vapour were theoretically predicted and experimentally confirmed, and therefore, features like melt solidification path, hydrogen production and melt oxidation are discussed.

13/00952 Characteristics of water vapor turbocompressors applied in refrigeration and heat pump systems

Šarevski, M. N. and Šarevski, V. N. *International Journal of Refrigeration*, 2012, 35, (5), 1484–1496.

Interdependence between centrifugal stage pressure ratio, peripheral Mach number and impeller peripheral speed, as well the influence of the refrigerating capacity on the dimensions of the centrifugal compressor are determined to obtain the range of reasonable usage of R718 refrigerating/heat pump systems. The deep vacuum operating conditions, the low specific volumetric cooling capacity of the R718 and the small molecular mass of the water are the peculiarities which determined the main parameters of the centrifugal compressor and the range of rational application of the R718 refrigerating/heat pump systems. The high peripheral impeller speed, high Mach number and high pressure ratio cause separated jet-wake flow and transonic flow phenomena in the compressor flow field. A method for prediction of the centrifugal compressor performance characteristics in variable working conditions (variable speed of rotation and variable inlet temperature) is presented. A decrease in the efficiency coefficient appears when the compressor works in conditions different to the design conditions, because of impeller/diffuser/volute optimal work conditions unadjustment, and because of transonic flow phenomena and choking flow, which may occur when the peripheral speed increases or/and inlet temperature decreases. Gas dynamic losses increase considerably if transonic flow phenomena appear. Occurrence of the supersonic flow in whole inlet region of the cascade causes choking flow and shock wave in the compressor flow field. The range of possible application of R718 centrifugal compressor refrigerating/heat pump units for air conditioning purposes is estimated to be very large, from tens of kW up to 1–2 MW. The estimated favourable range is 100–1200 kW.

13/00953 Characterizing metal-insulator-transition (MIT) phase change materials (PCM) for RF and DC micro-switching elements

Danner, B. L. *et al.* Coutu, R. A. *Procedia Engineering*, 2012, 47, 80–83.

Metal-insulator transition (MIT) phase-change materials (PCM) are material compounds that have the ability to be either conductors or insulators depending on external stimuli. A micromachined test structure for applying external electric fields across MIT wire segments was designed and fabricated. Using this novel test structure, germanium telluride (GeTe) and vanadium oxide (VOx) were successfully transitioned from a conductor to an insulator. The resistivity of the GeTe wire segments increased three to five orders of magnitude with ~40 V applied to the parallel plates of the test structure. The VOx wires exhibited an order of magnitude transition in resistivity with ~20 V applied. Characterization of both RF and DC switching performance of these MIT wire segments was completed and GeTe and VOx appear to be viable materials for micro-switching.

13/00954 Comparative study of working fluids for a Rankine cycle operating at low temperature

Vélez, F. *et al. Fuel Processing Technology*, 2012, 103, 71–77.

The main results of a thermodynamic study on the use of a low temperature heat source (150 °C as maximum) for power generation through a basic Rankine cycle are reported in this paper. Different working fluids such as water and some hydrocarbons and coolants are studied. The procedure consisted in modifying the input pressure and temperature to the turbine. The efficiency for these fluids is a weak function of temperature, i.e. overheating the inlet fluid to the turbine does not cause a significant change in the efficiency. However, when the pressure ratio in the turbine increases, much larger values of efficiency are obtained, and also, as the input temperature to the turbine rises, the efficiency increases more sharply. As result, a maximum efficiency of 9% was obtained. It is shown the technical viability of implementing this type of process for recovering residual wastes for very low temperature, as well as an energy alternative and/or strengthener of non-conventional energy sources in non-provided zones.

13/00955 Coupled electro-magneto-thermal model for induction heating process of a moving billet

Cho, K. H. *International Journal of Thermal Sciences*, 2012, 60, 195–204.

The purpose of this study is to present a coupled electro-magnetic and thermal model for numerical analysis of an induction heating system including the workpieces moving relative to the inductors. In this paper, a finite element method-based numerical analysis of a low-frequency (60 Hz) induction heating system for the one-dimensional solution of a stationary circular billet and the two-dimensional solution considering the dynamic effect of circular billets moving along the skid rails with constant speed are presented and compared against each other. The non-linearities of both the electromagnetic and thermal material properties are also taken into account in the model. The computational results have been compared with experimental data. As a result, it is suggested that the presented numerical model may be a very cost-effective tool in predicting the temperature of a workpiece in a variable flux field where the interested workpieces undergo an arbitrary change in the electro-magnetic fields. It is possible to obtain some preliminary results more accurate than those calculated from previous works using a stationary model on electromagnetic field and temperature distribution of workpieces by applying the presented numerical model.

13/00956 Cryogenic helium gas circulation system for advanced characterization of superconducting cables and other devices

Pamidi, S. *et al. Cryogenics*, 2012, 52, (4–6), 315–320.

A versatile cryogenic test bed, based on circulating cryogenic helium gas, has been designed, fabricated, and installed at the Florida State University Center for Advanced Power Systems. The test bed is being used to understand the benefits of integrating the cryogenic systems of multiple superconducting power devices. The helium circulation system operates with four sets of cryocooler and heat exchanger combinations. The maximum operating pressure of the system is 2.1 MPa. The efficacy of helium circulation systems in cooling superconducting power devices is evaluated using a 30-m-long simulated superconducting cable in a flexible cryostat. Experiments were conducted at various mass flow rates and a variety of heat load profiles. A one-dimensional thermal model was developed to understand the effect of the gas flow parameters on the thermal gradients along the cable. Experimental results are in close agreement with the results from the thermal model.

13/00957 Degradation of the performance of microchannel heat exchangers due to flow maldistribution

Nielsen, K. K. *et al. Applied Thermal Engineering*, 2012, 40, 236–247.

The effect of flow maldistribution on the performance of microchannel parallel plate heat exchangers is investigated using an established single blow numerical model and cyclic steady-state regenerator experiments. It is found that as the variation of the individual channel thickness in a particular stack (heat exchanger) increases the actual performance of the heat exchanger decreases significantly, deviating from the expected nominal performance. It is shown that this is due to both the varying fluid flow velocities in each individual channel and the thermal cross talk between the channels transverse to the direction of the flow.

13/00958 Design of condensation heat exchanger for the PAFS (passive auxiliary feedwater system) of APR+ (Advanced Power Reactor Plus)

Bae, B. U. *et al. Annals of Nuclear Energy*, 2012, 46, 134–143.

The APR+ (Advanced Power Reactor Plus), a next-generation nuclear power plant in Korea, has adopted the PAFS (passive auxiliary feedwater system) on the secondary system of the steam generator (SG) as an advanced safety feature. It is intended to replace the conventional auxiliary feedwater system, which consists of active components for the SG in a passive way. It removes decay heat from the reactor core by cooling down the secondary system of the SG using a condensation heat exchanger installed in the passive condensation cooling tank. The objective of this study is to design a condensation heat exchanger for the PAFS and to evaluate the cooling performance for the proposed design using the thermal hydraulic system analysis code, MARS (Multi-dimensional Analysis for Reactor Safety). Requirements such as the heat removal capacity and the prevention of water hammer were preferentially considered to determine the design parameters of the heat exchanger tube. The MARS code analysis result showed that the proposed design of the PAFS heat exchanger is able to cool down the required amount of decay heat. The distribution of a liquid volume fraction and flow regime predicted by the MARS code shows that the proposed design of the heat exchanger excludes the water hammer inside the tube. Estimation of a two-phase flow pressure drop indicates that the pressure drop inside the tube is negligible compared to the total pressure drop in the PAFS. From the MARS code analysis, it is concluded that the proposed design of the condensation heat exchanger in the PAFS satisfies the overall criteria for the performance of the passive heat removal system in APR+.

13/00959 Determining parameters of heat exchangers for heat recovery in a Cu–Cl thermochemical hydrogen production cycle

Rabbani, M. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11021–11034.

A heat exchanger is a device built for efficient heat transfer from one medium to another. Shell and tube heat exchangers are separated wall heat exchangers and are commonly used in the nuclear and process industry. The CuCl cycle is used to thermally crack water in to H_2 and O_2. The present study presents the heat exchanger thermal design using analysis of variance for heat recovery from oxygen at 500 °C, coming from the molten salt reactor. Polynomial regressions in terms of the amount of chlorine in the oxygen, the mass flow rate on the tube side, and the shell's outlet temperature are estimated for various exchanger parameters and the results are compared with the bell Delaware method. Based on energy and exergy analysis, this study also discusses the best possible path for the recovered heat from oxygen. Optimal heat exchanger parameters are estimated by Design-Expert® Stat-Ease for most effective heat recovery.

13/00960 Development of highly effective cryogenic printed circuit heat exchanger (PCHE) with low axial conduction

Baek, S. *et al. Cryogenics*, 2012, 52, (7–9), 366–374.

This paper presents the results of an experimental investigation of the thermal and hydraulic performance of a printed circuit heat exchanger (PCHE) for use in the cryogenic temperature region. Compact PCHEs with multiple corrugated, longitudinal flow microchannels were fabricated using chemical etching and diffusion bonding to evaluate their thermal and hydraulic performance. The testing of the PCHEs was conducted with helium gas at cryogenic temperatures. The pressure drop and thermal effectiveness values obtained from the measured pressures and temperatures are discussed. The thermal performance was predominantly affected by the axial conduction heat transfer in the low Reynolds number ranges of these experiments. A simple performance calculation model is presented, and the effectiveness calculated from the model is compared with the experimental data. The design of the cryogenic PCHE was then modified to reduce axial conduction losses.

13/00961 Dimensional optimization of microchannel heat sinks with multiple heat sources

Türkakar, G. and Okutucu-Özyurt, T. *International Journal of Thermal Sciences*, 2012, 62, 85–92.

Dimensional optimization of silicon microchannel heat sinks is performed by minimizing the total thermal resistance. Intel Core i7–900 desktop processor of chip core dimensions of 1.891 cm × 1.44 cm is considered as a reference processor which is reported to dissipate 130 W of heat. The properties are evaluated at the area weighted average of the fluid inlet and iteratively calculated outlet temperatures. The effects of the thermal and hydrodynamic entrance regions on heat transfer and flow are also investigated. The study is unique in that the optimization has been performed for localized multiple heat sources, as well as for a uniform heat load condition. The results of the optimization agreed very well with available ones in the literature.

13/00962 Direct and large eddy simulation of turbulent heat transfer at very low Prandtl number: application to lead–bismuth flows

Bricteux, L. *et al. Nuclear Engineering and Design*, 2012, 246, 91–97.

This paper deals with the issue of modelling convective turbulent heat transfer of a liquid metal with a Prandtl number down to 0.01, which is the order of magnitude of lead–bismuth eutectic in a liquid metal reactor. This work presents a DNS (direct numerical simulation) and a LES (large eddy simulation) of a channel flow at two different Reynolds numbers, and the results are analysed in the frame of best practice guidelines for RANS (Reynolds averaged Navier–Stokes) computations used in industrial applications. They primarily show that the turbulent Prandtl number concept should be used with care and that even recent proposed correlations may not be sufficient.

13/00963 Effect of silica dioxide particles on the evolution of biofouling by *Bacillus subtilis* in plate heat exchangers relevant to a heat pump system used with treated sewage

Tian, L. *et al. Chemical Engineering Journal*, 2012, 188, 47–56.

In 2008, a waste-heat utilization heat pump system was designed and constructed at the Beijing Olympic Village to use the energy in the treated sewage water (a bioenergy source) as a green approach for urban heat recovery. However, the treated sewage contains components that cause biofouling, such as heterotrophic bacteria, microbial nutrients and suspended substances (inorganic particles). The fouling deposited on the plate heat exchanger using the treated sewage as the heat transfer medium could sharply reduce by 60% the heat transfer coefficient in the plate heat exchanger within 40 days. Thus fouling is a composite material consisting of biological and inorganic substances. A novel combined plate heat exchanger and flow cell system was constructed to simulate the industrial treated sewage source heat pump system in the Olympic Village to better understand the biofouling characteristics. A plate heat exchanger was used to replace the actual plate heat exchangers with the same plate type, the same corrugation spacing between plates and the same material. Two flow cells with insertable studs were designed to simulate the flow in the plate heat exchanger. The effects of SiO_2, the most common inorganic particles in the treated sewage, on the biofouling of the heat exchanger surface were studied. The results showed that the SiO_2 particles influenced the biofilm development, further impacting the resulting heat transfer degradation. An increased biofouling mass was observed with increasing SiO_2 concentration; however, the highest organic substance level in the biofouling and the highest biofouling heat transfer resistance were achieved at intermediate SiO_2 particle concentrations. The inorganic particles led to expansion of the biofouling layer structure, which further affected the rate of biofouling buildup. Filaments and net biofouling structures were observed with the SiO_2 particles, leading to increased heat transfer resistance.

13/00964 Effective thermal conductivity of the heterogeneous lyophobic nanosystems for the usage in thermomechanical energy devices

Ievtushenko, O. V. *et al. International Journal of Thermal Sciences*, 2012, 62, 103–108.

This paper presents theoretical results of thermal conductivity of the heterogeneous lyophobic nanosystems characterized by structure that consists of interpenetrating components. More specifically, this structure is a liquid and a solid with communicating pores non-wet by the liquid. It has been shown in this paper that forced intrusion of liquid which takes place during compression of the system can be well described by using the model of intersecting pores.

13/00965 Experimental analysis and model validation of an opaque ventilated facade

López, F. P. *et al. Building and Environment*, 2012, 56, 265–275.

Natural ventilation is a convenient way of reducing energy consumption in buildings. In this study an experimental module of an opaque ventilated façade (OVF) was built and tested for assessing its potential of supplying free ventilation and air preheating for the building. A numerical model was created and validated against the experimental data. The experimental results showed that the flow rates induced in the façade cavity were due to mixed driving forces: wind and buoyancy. Depending on the weather conditions one of them was the main driving force, or both were of the same order. When the wind force was the main driving force, higher flow rates were found. In these cases buoyancy acted as supporting driving force. When the wind speed was low and buoyancy prevailed lower flow rates were found. Air and surface temperatures were predicted by the numerical model with a better accuracy than flow and energy rates. The model predicts correctly the influence of the wind and buoyancy driving forces. The experimental OVF module showed potential for free ventilation and air preheating, although it depends on weather and geometrical variables. The use of the numerical model using the right parameters was found viable for analysing the performance of an OVF.

13/00966 Experimental and numerical investigation into the hydrodynamics of nanofluids in microchannels

Singh, P. K. *et al. Experimental Thermal and Fluid Science*, 2012, 42, 174–186.

For this hydrodynamic study of nanofluids in microchannels, three microchannels of hydraulic diameters 130, 211 and 300 μm are fabricated by photolithographic and wet etching processes on silicon wafers. Alumina nanofluids with concentrations 0.25, 0.5 and 1.0 vol.% with particle sizes 45 and 150 nm are prepared, stabilized and characterized by standard methods like sonication, pH variation, transmission electron microscope and dynamic light scattering measurements. The base fluids used are water and ethylene glycol. The effect of volume fraction, channel size, particle size and base fluids are presented and analysed. It is shown that there is an early transition to turbulence for 211 and 301 μm channels. In addition, numerical modelling is carried out by using mixture rule and discrete phase modelling approach. This approach is found to be more suitable at higher Reynolds numbers whereas at lower Reynolds numbers the conventional mixture model can be used. Shear induced particle migration is identified to be an important phenomenon at higher Reynolds number and hence the reason for difference between these two models.

13/00967 Experimental and numerical studies on convective heat transfer from various urban canopy configurations

Pillai, S. S. and Yoshie, R. *Journal of Wind Engineering and Industrial Aerodynamics*, 2012, 104–106, 447–454.

This paper investigates the convective heat transfer coefficient (CHTC) variation of urban canopy surfaces for different urban canopy configurations by experimental and numerical simulation. The weather research forecasting (WRF) model coupled with the urban canopy model (UCM) is considered as an effective tool for prediction of urban heat island phenomena in urban areas. In the single layer UCM of WRF, the CHTC of urban canopy surfaces and its dependence on urban parameters such as building coverage ratio and building height variations are not explicitly modelled. In UCM, the CHTC of urban canopy surfaces are evaluated from Jürges relation. In this relation, the local CHTC from building walls and the ground depends only on the wind velocity inside the canopy. However, this cannot be justified since other urban parameters like building coverage ratio and building height variation also contribute to the CHTC of urban canopy surfaces. Moreover, Jürges relation cannot distinguish the difference between

CHTC of different building wall surfaces, i.e. windward, leeward and side walls, but expresses the CHTC for walls generally. In this study, wind tunnel experiments were firstly conducted to roughly grasp the dependence of urban parameters on bulk heat transfer from an urban canopy in a thermally stratified wind tunnel. However, it is not an easy task in wind tunnel experiments to evaluate local CHTC, which vary for individual canyon surfaces such as building roofs, walls and the ground. Numerical simulation validated by wind tunnel experiments can be an alternative for prediction of CHTC from building surfaces in an urban area. The authors conducted CFD simulation with a low-Reynolds number model to evaluate the CHTC from canopy surfaces. The calculated CFD results for velocity and temperature profile and bulk heat transfer from an urban canopy showed good agreement with experimental results. After this validation, the effects of urban canopy parameters on local convective heat transfer on individual surfaces were investigated by CFD simulation. Based on these results, the CHTC will be modified with respect to urban parameters, and will be incorporated into the UCM of the WRF model in a future study.

13/00968 Experimental investigation of a heat switch based on the precise regulation of a liquid bridge

Jeong, S. H. *et al. Applied Thermal Engineering*, 2012, 39, 151–156.

Thermal management is a key issue in various fields of engineering. The effective counterplan has to be come up with for achieving high thermal stability suitable for thermally sensitive system. Here, the concept utilizing a liquid-based heat switching method was presented as one of the promising solutions in the thermal management, and the proposed system is composed of a hot plate, cold plate, fluid chamber and actuator. The heat switching works by means of controlling the formation of the liquid bridge between the two plates, and it enables to not only control the thermal resistance but also distribute the heat to the surroundings using the liquid bridge. Thus, the thermal performance of the proposed heat switch highly depends on the formation and motion of the liquid bridge. Empirically, the optimal geometry of the heat switch, the diameter of the liquid channel and clearance between two plates, was determined to be suitable for creating and rupturing the liquid bridge. To investigate the effects of its geometry, the pressure analysis and observation of the liquid bridge through CCD were conducted, respectively. The constructed heat switching system was applied to the LED-based testing module to control the LED junction temperature regulation and thermal resistance between the LED plate and the heat sink. As a result, the behaviour of the liquid bridge and its effect on the heat switching were empirically understood.

13/00969 Experimental investigation of the influence of different leaking gases on the heat transfer in a HVMLI cryogenic tank after SCLIV

Zhu, M. and Wang, R. S. *Cryogenics*, 2012, 52, (7–9), 331–335.

This paper presented an experimental investigation of the influence of different leaking gases on the heat transfer process in a high-vacuum-multilayer-insulation cryogenic tank after sudden catastrophic loss of insulation vacuum. The experiments were conducted with the break-down of the insulation vacuum with nitrogen, air, helium, oxygen, argon, carbon dioxide and the gas mixture of argon and carbon dioxide. The maximum value of the venting rate and heat flux could be ordered as following: $CO_2 > O_2 > Ar >$ the gas mixture $> He > Air > N_2$, while the average value of the venting rate and heat flux could be ordered as following: $O_2 > Ar > He >$ the gas mixture $> CO_2 > Air > N_2$. The temperature distribution indicated that phase change heat transfer happened in the insulation jacket after the five different gases including air, argon, the gas mixture of argon and carbon dioxide, oxygen and carbon dioxide were introduced into the insulation jacket.

13/00970 Experimental investigation of thermoelectric power generation versus coolant pumping power in a microchannel heat sink

Rezania, A. *et al. International Communications in Heat and Mass Transfer*, 2012, 39, (8), 1054–1058.

The coolant heat sinks in thermoelectric generators (TEG) play an important role in order to power generation in the energy systems. This paper explores the effective pumping power required for the TEGs cooling at five temperature difference of the hot and cold sides of the TEG. In addition, the temperature distribution and the pressure drop in sample microchannels are considered at four sample coolant flow rates. The heat sink contains 20 plate-fin microchannels with hydraulic diameter equal to 0.93 mm. The experimental results show that there is a unique flow rate that gives maximum net-power in the system at the each temperature difference.

13/00971 Experimental study on an inverter heat pump with HFC125 operating near the refrigerant critical point

Wang, F. *et al. Applied Thermal Engineering*, 2012, 39, 1–7.

An experimental study on an inverter heat pump with HFC125 operating near the refrigerant critical point was carried out. The coefficient of performance (COP) and exergy efficiency of the system were investigated under different compressor speed, water flow rate and different hot water temperatures of the condenser. The exergy defect in each component was determined. The results show that the exergy efficiency of the system increases initially and then decreases while the COP constantly decreases with the increase of the temperature of hot water. The results of this study can provide useful guidelines for optimal design and operation of this type of heat pump system in its present or future applications.

13/00972 Forced convective mixing in a zero boil-off cryogenic storage tank

Ho, S. H. and Rahman, M. M. *International Journal of Hydrogen Energy*, 2012, 37, (13), 10196–10209.

This paper presents the results of a study of fluid flow and heat transfer of liquid hydrogen in a cryogenic storage tank with a heat pipe and an array of pump-nozzle units. A forced flow is directed onto the evaporator section of the heat pipe to prevent the liquid from boiling off when heat leaks through the tank wall insulation from the surroundings. An axisymmetric computational model was developed for the simulation of convective heat transfer in the system. Steady-state velocity and temperature fields were solved from this model by using the finite element method. Forty-five configurations of geometry and velocity were considered. As the nozzle fluid speed increases, the values of the maximum, average, and spatial standard deviation of the temperature field decrease non-linearly. Parametric analysis indicates that overall thermal performance of the system can be significantly improved by reducing the gap between the nozzle and the heat pipe, while maintaining the same fluid speed exiting the nozzle. It is also indicated that increased inlet tube length of the pump-nozzle unit results in slightly better thermal performance. Increased heat pipe length also improves thermal performance but only for low fluid speed.

13/00973 Fully coupled heat conduction and deformation analyses of nonlinear viscoelastic composites

Khan, K. A. and Muliana, A. H. *Composite Structures*, 2012, 94, (6), 2025–2037.

This study presents an integrated micromechanical model-finite element framework for analysing coupled heat conduction and deformations of particle-reinforced composite structures. A simplified micromechanical model consisting of four sub-cells, i.e. one particle and three matrix sub-cells is formulated to obtain the effective thermomechanical properties and micro–macro field variables due to coupled heat conduction and non-linear thermoviscoelastic deformation of a particulate composite that takes into account the dissipation of energy from the viscoelastic constituents. A time integration algorithm for simultaneously solving the equations that govern heat conduction and thermoviscoelastic deformations of isotropic homogeneous materials is developed. The algorithm is then integrated to the proposed micromechanical model. A significant temperature generation due to the dissipation effect in the viscoelastic matrix was observed when the composite body is subjected to cyclic mechanical loadings. Heat conduction due to the dissipation of the energy cannot be ignored in predicting the factual temperature and deformation fields within the composite structure, subjected to cyclic loading for a long period. A higher creep resistant matrix material or adding elastic particles can lower the temperature generation. The analyses suggest that using particulate composites and functionally graded materials can reduce the heat generation due to energy dissipation.

13/00974 Heat exchanger network synthesis using a stagewise superstructure with non-isothermal mixing

Huang, K. F. *et al. Chemical Engineering Science*, 2012, 73, 30–43.

Much work on heat exchanger network synthesis (HENS) via mathematical programming has employed a stagewise superstructure with the assumption of isothermal mixing. It is well known that the superstructure may miss potentially better networks. This article proposes a mixed-integer non-linear programming formulation and a solution strategy to incorporate non-isothermal mixing in HENS. The authors use an existing modification of the stagewise superstructure, propose novel and improved temperature bounds, and propose logical constraints to obtain superior HENs. Using several examples, this approach is shown to find superior networks compared to those known in the literature, especially for larger and more difficult problems. Furthermore, the authors propose exact approaches for handling log-mean temperature difference (LMTD) without numerical difficulty, and compare the effectiveness of the known LMTD approximations. They also show that including the stage bypass variables and constraints improves solution quality and efficiency.

13/00975 Heat transfer analysis and experimental verification of casted heat exchanger in non-icing and icing conditions in winter

Yu, J. *et al. Renewable Energy*, 2012, 41, 39–43.

Seawater-source heat pump systems (SWHP) are recognized to be outstanding heating, cooling and water heating systems. A large number of SWHP systems have been used in residential and commercial buildings in coastal areas due to the attractive advantages of high efficiency and environmental friendliness. In this paper, two mathematical models that described heat transfer process of casted heat exchanger (CHE) adopted by SWHP systems in the icing and non-icing conditions in winter have been developed and validated by an experimental study. The CHE is consisted of pipes immersed in the seawater and used for transferring heat between the seawater and the heat exchanger pipes of the SWHP. In addition, a computer code has been implemented to simulate the effects of flow rate of the secondary refrigerant, length of the CHE and the temperature of the seawater on the heat transfer performance. The effect of the ice outside the pipe due to the low seawater temperature on heat transfer has been discussed and the comparison of the heat transfer rate in two conditions demonstrates that the effect of icing on heat transfer performance is great. As a result, application of SWHP systems with CHE in coastal areas in China is feasible due to the favourable geographical conditions and environment.

13/00976 Heat transfer augmentation by helically twisted tapes as swirl and turbulence promoters

Eiamsa-ard, S. *et al. Chemical Engineering and Processing: Process Intensification*, 2012, 60, 42–48.

This paper describes heat transfer enhancement attributed to helically twisted tapes (HTTs). Each helically twisted tape was fabricated by twisting a straight tape to form a typical twisted tape then bending the twisted tape into a helical shape. The experiments were performed using HTTs with three twist ratios (y/W) of 2, 2.5 and 3, three helical pitch ratios (p/D) of 1, 1.5 and 2 for Reynolds number between 6000 and 20,000. The conventional helical tape (CHT) was also tested for comparison. The obtained results reveal that at similar conditions (y/W and p/D), HTTs give lower Nusselt number and friction but higher thermal performance factor than CHTs. Heat transfer rate and friction factor increase as the tape twist ratio and helical pitch ratio decrease, while the thermal performance shows opposite trend. In the present range, the highest thermal performance factor of 1.29 is achieved by utilizing the tape with the largest twist ratio ($y/W = 3$) and helical pitch ratio ($p/D = 2$) at Reynolds number of 6000.

13/00977 Heat transfer characteristics of a helical heat exchanger

San, J. Y. *et al. Applied Thermal Engineering*, 2012, 39, 114–120.

Heat transfer performance of a helical heat exchanger was investigated. The heat exchanger is composed of a helical tube with rectangular cross-section and two cover plates. The ε–Ntu relation of the heat exchanger was obtained using a numerical method. In the analysis, the flow in the tube (helical flow) was considered to be mixed and the flow outside the tube (radial flow) was unmixed. In the experiment, the Darcy friction factor (f) and convective heat transfer coefficient (h) of the radial flow were measured. The radial flow was air and the helical flow was water. Four different channel spacing (0.5, 0.8, 1.2 and 1.6 mm) were individually considered. The Reynolds numbers were in the range 307–2547. Two correlations, one for the Darcy friction factor and the other for the Nusselt number, were proposed.

13/00978 Heat transfer enhancement by spinodal decomposition in micro heat exchangers

Farisè, S. *et al. Experimental Thermal and Fluid Science*, 2012, 42, 38–45.

This study investigates experimentally how the heat transfer in a laminar flow can be enhanced by using a partially miscible binary liquid–liquid mixture undergoing spinodal decomposition. A mixture of acetone–hexadecane is quenched in a micro heat exchanger to induce spinodal decomposition. The heat transfer rate is enhanced by self-induced convective effects sustained by the free energy liberated during phase separation. The authors report a heat-transfer augmentation of up to 150% when phase separation occurs in microchannels. Since acetone and hexadecane are immiscible below a critical temperature of 27 °C, to obtain their spinodal decomposition the mixture inlet temperature are above 27 °C and the heat exchangers wall are well below. The authors measured the heat transfer with a feedback method instead of a direct measure. To validate this measuring technique they carefully verified the energy balance. They then fabricated a copper single-channel heat sink and two different types of multi-channel array. The single-channel exchanger allowed them to visualize the induced convection. The arrays of microchannels promise to achieve very high heat transfer coefficients with small flow rate.

13/00979 Heat transfer enhancement in double-pipe heat exchanger by means of rotor-assembled strands

Zhang, Z. *et al. Chemical Engineering and Processing: Process Intensification*, 2012, 60, 26–33.

Thermo-hydraulic characteristics of turbulent flow in plain tube equipped with rotor-assembled strands of different geometries and leads were reported, ahead of which an experiment considering a smooth tube had been conducted to calibrate the experimental system and data reduction method. The effects of rotor lead on heat transfer and friction characteristics were emphasized consequently. Experimental results revealed that rotor-assembled strands of different geometries employed improved heat transfer significantly with Nusselt number increased by 71.5–123.1% and friction factor increased by 37.4–74.8% compared with plain tube. There into, the helical blade rotor brought the most augmentation of heat transfer, while the blade-discreted rotor caused the largest friction loss. Generally considering, helical blade rotor with ladders offered first-class performance sequentially followed by helical blade rotor and blade-discreted rotor. For helical blade rotor with ladders, Nusselt number and friction factor both increased with the decrease of rotor lead. The best thermal performance factor was achieved when helical blade rotor with ladders was manufactured with certain parameters (rotor diameter is 22 mm, rotor lead is 150 mm). At last, the correlations of experimental results were presented based on thorough multivariate linear normal regression method.

13/00980 Heat transfer of pulsating turbulent pipe flow in rolling motion

Yan, B. H. *et al. Progress in Nuclear Energy*, 2012, 59, 59–65.

The heat transfer of turbulent pulsating flow is of vital importance in nuclear reactor thermal hydraulic analysis in ship motions. In this paper, the heat transfer behaviour of turbulent pulsating flow is analysed. The calculation results are verified with experimental data, with satisfactory agreement obtained. The effect of span-wise and transverse additional forces decreases with Reynolds number increasing and is significant in low Reynolds number. The effect of velocity oscillation period on the heat transfer is more limited than the effect of Reynolds number and oscillating velocity Reynolds number.

13/00981 Innovative production of nuclear fuel by microwave internal gelation: heat transfer model of falling droplets

Cabanes-Sempere, M. *et al. Progress in Nuclear Energy*, 2012, 57, 111–116.

Based on closed packed microspheres produced by internal gelation, the Sphere-pac concept provides a safer and cleaner process and better remote production capability compared to the traditional production of nuclear fuels. Whereas classical reactor fuel rods are fed with UO_2 pellets, this advanced concept is suggested for minor actinide bearing fuels. This paper focuses on the thermal analysis of the microspheres during their preparation by microwave-assisted internal gelation (MIG). Internal gelation is a sol-gel process initiated by a temperature shift within aqueous droplets. Alternatively this critical temperature increase takes place by contact heat transfer from a hot silicon-oil bath. Microwave heating of the droplets during their free fall provides a simpler and cleaner process, where the experimental parameters have to be carefully optimized. A MATLAB model is developed to study the thermal behaviour of a droplet during processing inside a microwave resonant cavity. Several analytical calculations were to evaluate the model and to optimize the upcoming experimental conditions. Parameter variations contribute to a better knowledge and understanding of the energy transfer between the drops and the electromagnetic field that is used for the determination of the best frequency and the design of the microwave cavity. The model plus the case studies lead to the conclusion, that in this application the best possible energy transfer efficiency is required to achieve the necessary temperature increase in the very short residence time. According to literature the best energy transfer efficiency is achieved with a frequency of 12 GHz in the X-band. At this frequency a generator power of 100 W is sufficient to cause an 80 K temperature increase and therefore to trigger the gelation.

13/00982 Inverse determination of building heating profiles from the knowledge of measurements within the turbulent slot-vented enclosure

Liu, D. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4597–4612.

Slot ventilated enclosure flows have been simulated, respectively in displacement ventilation and mixed ventilation covering from the forced convection dominated flow to the natural convection dominated flow. Direct convection simulation together with the turbulent streamlines and turbulent heatlines demonstrate that the enclosure flow pattern, indoor thermal level and heat transfer potential will depend on the interactions of external forced flow and thermal buoyancy driven flows, i.e. Reynolds number and Grashof number. In subsequent inverse convection modelling, the inverse determination of enclosure wall heat flux profiles was conducted by the use of adjoint methodology, in which the direct, sensitivity and adjoint problems are formulated and solved by finite volume method. The effects of the supplying air flow rate, thermal source strength, ventilation mode, flux functional forms, and the measurement errors on the accuracy of inverse turbulent convection estimation have been investigated. The inverse solutions of turbulent convections are of low level accuracy as the flow becomes thermal-driven turbulent flows, and they deteriorate as the noise levels increase. This work is of fundamental importance for the room air flow design and measurements involving the turbulent thermal convections.

13/00983 Investigations of the conjugate heat transfer and windage effect in stepped labyrinth seals

He, K. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4536–4547.

In the current paper, conjugate heat transfer and windage heating in the stepped labyrinth seals with smooth and honeycomb lands are numerically investigated by using the commercial software ANSYS CFX11.0. Firstly, the utilized numerical approaches, such as the turbulence model and grid independence analysis, are determined to ensure a suitable numerical method for the present study. Based on the obtained measurement data, the computed heat transfer coefficients on the rotor and stator surfaces are carefully validated. To reveal the influence of the solid domain on the heat transfer computations, the comparisons between the results with and without solid domain are performed. It shows that the predicted heat transfer coefficient distributions with the presented conjugate heat transfer methods (with solid domain) agree well with the experimental data. Difference between the numerical results with and without solid domain only exists in the high temperature gradient region. Compared to the smooth labyrinth seal, the presence of honeycomb cells increases the temperature gradient in the labyrinth fin (solid domain) and significantly decreases the temperature gradient in the stator (solid domain). Secondly, in order to assess the influence of the rotating effect on the windage heating for the stepped labyrinth seal, total temperature difference between the seal inlet and outlet are computed under different effective pressure ratios for both the smooth and honeycomb configurations. Based on the energy conservation law, the windage loss for the high speed rotating seal is also obtained by taking the heat transfer between the fluid and solid into consideration. Finally, the influences of the effective pressure ratio and inlet preswirl ratio on the heat transfer coefficient distributions of rotor and stator for both the smooth and honeycomb configurations are discussed in detail.

13/00984 Launch ascent testing of a representative Altair ascent stage methane tank

Johnson, W. L. *et al. Cryogenics*, 2012, 52, (4–6), 278–282.

In order to support long duration cryogenic propellant storage, NASA is investigating the long-duration storage properties of liquid methane. The methane lunar surface thermal control (MLSTC) testing is using a tank of the approximate dimensions of the Altair lunar ascent propellant tanks. The tank was insulated with multilayer insulation and placed inside of a vacuum chamber to simulate the various environments that would be encountered during launch and travel from Earth to the lunar surface, including long duration stays on the lunar surface. One of these environments to be studied is the launch and ascent environment; while all the effects of this mission phase cannot be simulated at the same time, an effort was made to simulate as many as possible. Boil-off testing included ambient pressure ground hold testing followed by a rapid depressurization of the vacuum chamber during which the liquid methane tank was allowed to come to steady state condition in the high vacuum environment. The data gathered from the series of tests fit within pre-test predictions and yielded much needed test data for rapid depressurization using liquid methane.

13/00985 Minimization of mass for heat exchanger networks in spacecrafts based on the entransy dissipation theory

Xu, Y. C. and Chen, Q. *International Journal of Heat and Mass Transfer*, 2012, 55, (19–20), 5148–5156.

Mass reduction strongly contributes to reduce the cost and promote the performance of spacecraft. During the design of spacecraft, mass minimization for the heat exchanger networks (HENs) is a fundamental and attractive issue for which series of global optimization methods based on numerical simulation have been applied. However, among the existing methods, there is not yet a theoretical method. To develop a theoretical approach, the authors introduce the concept of entransy dissipation in this work, analyse the entransy dissipation of each heat transfer process and eventually derive the expressions of the total entransy dissipation in the heat exchanger networks, which helps to establish the direct theoretical relation between all the design parameters, i.e. the areas of radiator and heat exchangers and heat capacity rates of each fluids, and the known conditions, i.e. the released heat and inlet temperature of fluid. With the relation, the optimization problem is successfully solved with conditional extremum model. Finally, through the application in a typical heat exchanger network, the authors prove the optimized total mass to be the least, and find that: (1) the total mass increases with the released heat; and (2) the working fluids with larger ρc_p^3 lead to less mass and energy consumption of HENs.

13/00986 Numerical investigation of heat transfer enhancement in ribbed channel for the first wall of DFLL-TBM in ITER

Jin, Q. *et al. Fusion Engineering and Design*, 2012, 87, (7–8), 974–978.

As an important component of Dual Functional Lithium Lead-Test Blanket Module (DFLL-TBM), the first wall (FW) must withstand and remove the heat flux from the plasma ($q'' = 0.3\,\mathrm{MW/m^2}$) and high nuclear power deposited in the structure at normal plasma operation scenario of ITER. In this paper the transverse ribs arranged along the plasma facing inner wall surface were used to enhance the heat transfer capability. After the validation compared with empirical correlations the Standard k–ω model was employed to do the numerical simulation using FLUENT code to investigate the heat transfer efficiency and flow performance of coolant in the ribbed channel preliminarily. The perforation on the bottom of rib was proposed near the lower heat transfer area (LHTA) to improve the heat transfer performance according to results of analyses.

13/00987 Numerical modeling of an ITER type cryopump

Varoutis, S. and Day, C. *Fusion Engineering and Design*, 2012, 87, (7–8), 1395–1398.

The present article is focused on the computational investigation of a two-dimensional axisymmetric complex geometry of a model cryopump by the direct simulation Monte Carlo (DSMC) method. Since the flow close to the cryopanels can be assumed free molecular due to low pressures, the capture coefficient of the cryopanels can be estimated by applying the test particle Monte Carlo method. Then, this information can be used as input data to the corresponding DSMC simulations. The macroscopic parameters of practical interest as the bulk velocity, the pressure and the temperature in the whole flow field have been calculated as functions of the incoming gas throughput and of the pump inlet valve position. The importance of these calculations is based on the fact that it can provide information for quantities which are not accessible for measurement during pump operation and that it can be used for prediction of the pump behaviour. This paper describes a post-operational investigation of a built pump and is thought as a proof-of-principle test to include this approach in the design process of a future pump development. Finally, the presented code could be further developed and benchmarked towards the control of the final pump as installed in ITER.

13/00988 Numerical study of flow and heat-transfer characteristics of cryogenic slush fluid in a horizontal circular pipe (SLUSH-3D)

Ohira, K. *et al. Cryogenics*, 2012, 52, (7–9), 428–440.

Cryogenic slush fluids, such as slush hydrogen and slush nitrogen, are two-phase, single-component fluids containing solid particles in a liquid. Since their density and refrigerant capacity are greater than those of liquid-state fluids alone, there are high expectations for use of slush fluids as functionally thermal fluids in various applications, such as fuels for spacecraft engines, clean energy fuels to improve the efficiency of transportation and storage, and as refrigerants for high-temperature superconducting equipment. In this research, a three-dimensional numerical simulation code (SLUSH-3D), including the gravity effect based on the thermal non-equilibrium, two-fluid model, was constructed to clarify the flow and heat-transfer characteristics of cryogenic slush fluids in a horizontal circular pipe. The calculated results of slush nitrogen flow performed using the numerical code were compared with the authors' experimental results obtained using the PIV method. As a result of these comparisons, the numerical code was verified, making it possible to analyse the flow and heat-transfer characteristics of slush nitrogen with sufficient accuracy. The numerical results obtained for the flow and heat-transfer characteristics of slush nitrogen and slush hydrogen clarified the effects of the pipe inlet velocity, solid fraction, solid particle size, and heat flux on the flow pattern, solid-fraction distribution, turbulence energy, pressure drop, and heat-transfer coefficient. Furthermore, it became clear that the difference of the flow and heat-transfer characteristics between slush nitrogen and slush hydrogen were caused to a large extent by their thermo-physical properties, such as the solid–liquid density ratio, liquid viscosity, and latent heat of fusion.

13/00989 Preparation, characterization and thermal properties of micro-encapsulated phase change materials

Pan, L. *et al. Solar Energy Materials and Solar Cells*, 2012, 98, 66–70.

In this study, a novel microencapsulated phase change material (palmitic acid@AlOOH) was prepared using an *in situ* emulsion interfacial poly-condensation method. The resulting colloidal-sphere microcapsules, with diameter around 200 nm, are of core-shell microstructures. Characteristic peaks of both palmitic acid and AlOOH can be observed during their infrared spectrum characterization. According to the TGA examinations, the encapsulated ratios of palmitic acid (PA) to PA@AlOOH are 52%, 57% and 69%. The DSC results indicate that melting temperatures of the microencapsulated PCMs are remarkably 50 °C lower than those of pristine PA, which might originate from the strong interface interactions between the core and shell of PA@AlOOH. The thermal storage capabilities of the microcapsules are also tested. The method and mechanism of this study can be extended to design other organics@inorganics PCMs with different core-shell structured compositions.

13/00990 Pressure and temperature transients of a cryogenic distillation system during abnormal operation or accidents

Ana, R. G. and Draghia, M. *Fusion Engineering and Design*, 2012, 87, (5–6), 543–546.

Cryogenic distillation system (CDS) is being employed, among other applications, in tritium separation technologies. CDS in combination with a liquid phase catalytic exchange (LPCE) process or with a combined electrolytic catalytic exchange (CECE) process is used for tritium removal/recovery from tritiated water. Large amounts of tritiated water can be produced during long time operation of CANDU reactors or in case of ITER mainly by the detritiation system (DS). The CDS used to remove/recover tritium consists of a cascade of cryogenic distillation columns and a refrigeration unit which provides the cooling capacity for the condensers of CD columns. The columns, together with the condensers and the process heat-exchangers are accommodated in a vacuum insulated cold box. During abnormal events or accidents, significant amount of liquid hydrogen–deuterium–tritium or helium refrigerant can be spilt inside the cold box or even into the building. The paper analyses some critical scenarios due to single failure mode or various combinations of failures such as: loss of refrigerant in the columns; loss of vacuum insulation; process liquid spilt into the cold box; refrigerant fails into cryogenic distillation columns. The study presented in the paper is concerning to Tritium Removal Facility from NPP Cernavoda but gives information and some references for the methodology that can be implemented for ITER Isotope Separation System.

13/00991 Refrigerant-based measurement method of heat pump seasonal performances

Tran, C. T. *et al. International Journal of Refrigeration*, 2012, 35, (6), 1583–1594.

There is no reliable measurement method of air-to-air heat pump seasonal performances. This study tested a method based on intrusive measurements on the refrigerant side. The method proposed uses two Coriolis mass flow meters for the measurement of the refrigerant flow rate and of the vapour quality at the indoor heat exchanger outlet. The method is validated by testing an air-to-water heat pump in laboratory conditions and by using the water enthalpy method as a reference. Results confirm that the refrigerant density measurement with a Coriolis flow meter can help to predict the refrigerant vapour quality with satisfactory accuracy if the quality is not too high. The method is also reliable in dynamic conditions (including for defrosting periods). It will then be used as a reference to check the accuracy of different *in situ* measurement methods for air-to-air heat pumps.

13/00992 Russian development of enhanced heat flux technologies for ITER first wall

Mazul, I. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 437–442.

Recently the ITER first wall (FW) design has been significantly upgraded to improve resistance to electromagnetic loads, to facilitate FW panel replacement and to increase FW ability to withstand higher (up to 5 $\mathrm{MW/m^2}$) surface heat loads. The latter has made it necessary to re-employ technologies previously developed for the now-abandoned port limiters. These solutions are related to the cooling channel with CuCrZr–SS bimetallic walls and hypervapotron-type cooling regime, optimization of Be-tiles dimensions and Be to CuCrZr joining technique. A number of representative mockups were tested at high heat flux (HHF) at the Tsefey electron-beam facility to verify the thermo-hydraulic characteristics of the reference cooling channel design at moderate water flow velocities ($V = 1$–3 m/s, $P = 2$–3 MPa, $T = 110$–170 °C). The heat flux was gradually varied in the range of 1–10 $\mathrm{MW/m^2}$ until the critical heat flux was registered. The mockups of hypervapotron structure demonstrated the required cooling efficiency and critical heat flux margin (1.4) at a water velocity of ≥ 2 m/s. Dimensions of Be armor tiles strongly affect the thermo-mechanical stresses both in the CuCrZr cooling wall and at the Be–CuCrZr interface. Results of tile dimensions optimization (variable in the range $12\,\mathrm{mm} \times 12\,\mathrm{mm} \times 6$ to $50\,\mathrm{mm} \times 50\,\mathrm{mm} \times 8\,\mathrm{mm}$) obtained by the HHF (variable in the range of 3–8 $\mathrm{MW/m^2}$) experiments are presented and compared with analysis. It is shown that optimization of the tile geometry and joining technology provides the required cyclic fatigue lifetime of the reference FW design.

13/00993 Simulation of the future performance of low-energy evaporative cooling systems using UKCP09 climate projections

Hanby, V. I. and Smith, S. Th. *Building and Environment*, 2012, 55, 110–116.

Recent activity in the development of future weather data for building performance simulation follows recognition of the limitations of traditional methods, which have been based on a stationary (observed) climate. In the UK, such developments have followed on from the availability of regional climate models as delivered in UKCIP02 and recently the probabilistic projections released under UKCP09. One major area of concern is the future performance and adaptability of buildings which employ exclusively passive or low-energy cooling systems. One such method which can be employed in an integral or retrofit situation is direct or indirect evaporative cooling. The effectiveness of evaporative cooling is most strongly influenced by the wet-bulb depression of the ambient air, hence is generally regarded as most suited to hot, dry climates. However, this technology has been shown to be effective in the UK, primarily in mixed-mode buildings or as a retrofit to industrial/commercial applications. Climate projections for the UK generally indicate an increase in the summer wet-bulb depression, suggesting an enhanced potential for the application of evaporative cooling. The paper illustrates this potential by an analysis of the probabilistic scenarios released under UKCP09, together with a detailed building/plant simulation of case study building located in south-east England. The results indicate a high probability that evaporative cooling will still be a viable low-energy technique in the 2050s.

13/00994 Study on a snow storage system in a renovated space

Hamada, Y. *et al. Renewable Energy*, 2012, 41, 401–406.

This paper proposes a snow storage system in a renovated space for efficient energy use and reduction of the costs related to snow utilization, and aims to clarify the system's effectiveness. First, it gives an outline of the system together with a description of the facility used for demonstration testing. Second, it highlights the results of long-term measurements relating to snow storage characteristics, which showed that 59% of the latent energy in the initially stored snow had been used for cooling by the end of the relevant period. The authors discuss how heat balance analysis revealed a relatively high level of heat loss from the floor due to the storage facility's location in an underground space, and confirm that the system has the potential to secure a high level of energy conservation. Finally, the paper outlines the results of analysis conducted throughout the construction and operation phases of the cooling system, which revealed that the initial cost was 96% that of a conventional cooling system.

13/00995 Subcooled and saturated boiling of ammonia–lithium nitrate solution in a plate-type generator for absorption machines

Venegas, M. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4914–4922.

This paper presents the experimental heat transfer evaluation during subcooled and saturated boiling of ammonia–lithium nitrate solution in a fusion plate heat exchanger, acting as a vapour generator under operating conditions representative of single-effect absorption machines. The solution flow rate and outlet temperature were modified in the ranges of 0.041–0.083 kg/s and 78–97 °C, respectively. The region where vapour bubbles begin to arise is estimated using a correlation for the wall superheat required for the onset of nucleate boiling. Results show that subcooled boiling is present in the generator. The initial boiling temperature is about 3.1 °C lower than the saturation temperature. The influence of the heat and mass fluxes on the boiling heat transfer coefficient is analysed. The paper offers a correlation for the Nusselt number, including the subcooled and saturated boiling regions.

13/00996 The energy consumption performance of roof lawn gardens in Thailand

Permpituck, S. and Namprakai, P. *Renewable Energy*, 2012, 40, (1), 98–103.

Statistics have confirmed that a lawn placed on a roof top can reduce the cooling load. In this study, the VISUAL DOE 4.0 energy simulation program was used to determine the effects of roof lawn gardens (RLG) on the annual energy required for cooling, and annual electrical usage in an experimental model. The overall heat transfer coefficient (U-value) of the RLG was estimated by using data from site measurements and the effect of the RLG on the building's energy consumption was calculated by the simulation program. The effect of different thicknesses of soil was also investigated. From the field measurements, it was confirmed that the RLG could reduce building heat gain. Thus, an experiment was set up to find the energy benefits of the RLG. With evaporative cooling by the RLG, it was found that the consumption of energy in a building with a RLG with 0.20 m of soil was

37.11% less than in a building with a bare roof surface (without evaporative cooling). Moreover, a building with 0.10 m of soil in the RLG consumed 31.07% less energy than a building with a bare roof surface. The results show that an increase in the thickness of the soil layer reduces the building energy consumption.

13/00997 Tools for designing the cooling system of a proton exchange membrane fuel cell

Soupremanien, U. *et al. Applied Thermal Engineering*, 2012, 40, 161–173.

Proton exchange membrane fuel cell (PEMFC) requires a careful management of the heat distribution inside the stack. The proton exchange membrane is the most sensitive element of this thermal management and it must operate under specific conditions in order to increase the lifetime and also the output power of the fuel cell. These last decades, the enhancement of the output power of the PEMFC has led the manufacturers to greatly improve the heat transfer effectiveness for cooling such systems. In addition, homogenizing the bipolar plate temperature increases the lifetime of the system by limiting the occurrence of strong thermal gradients. In this context, using a fluid in boiling conditions to cool down the PEMFC seems to be very suitable for this purpose. In order to compare the thermal performances between a coolant used in single-phase flow or in boiling flow conditions, the authors have built an experimental set-up allowing the investigation of cooling flows for these two conditions. Moreover, the geometry of the cooling channels is one of the key parameters which allows the improvement of the thermal performances. Indeed, the size or the aspect ratio of these channels could be designed in order to decrease the thermal system response. The sizing of the fuel cell cooling system is of paramount importance in boiling flow conditions because it can modify, not only the pressure losses along the channel and the heat transfer coefficient like in a single-phase flow but also, the onset of nucleate boiling and the dryout point or critical heat flux. Thus, in order to understand some heat transfer mechanisms, which are geometry-dependent, a parametric study was completed by considering flows in four different rectangular channels. Finally, this study allows a better insight on the optimization of the geometrical parameters which improve the thermal performances of a PEMFC, from a cooling strategy aspect point of view.

11 ENGINES

Power generation and propulsion, electrical vehicles

13/00998 An extended multi-regime flamelet model for IC engines

Mittal, V. *et al. Combustion and Flame*, 2012, 159, (8), 2767–2776.

Modelling internal combustion engines is challenging due to the various coupled multi-physics phenomena. With the advent of modern supercomputing and advanced modelling techniques, studying and designing these engines through detailed simulations is becoming tractable. Since the combustion process is the primary controlling feature in these engines, a high fidelity combustion model is essential. This model must be efficient and valid across different combustion regimes, since modern engines might operate in hybrid modes. The representative interactive flamelet combustion model is a possible choice. This model has been developed to describe ignition, combustion, and pollutant formation in direct-injected diesel engines. However, it has recently been shown that the model has the correct asymptotic behaviour for both diesel and homogeneous charge compression ignition (HCCI) regimes, and the model has been applied successfully for HCCI-type combustion. In this study, the model is validated against two-dimensional direct numerical simulation data with multi-step finite rate chemistry to evaluate model performance in the diesel, the HCCI, and hybrid regimes. A wide range of temperature and mixture fraction stratification cases are simulated to evaluate the model performance across different modes. The model performs well for all cases considered, even when high levels of concurrent thermal and charge stratification are present.

13/00999 Application of in situ oxidation-resistant coating technology to a home-made 100 kW class gas turbine and its performance analysis

Kim, M. T. and Lee, S. W. *Applied Thermal Engineering*, 2012, 40, 304–310.

An axial type 100 kW class gas turbine power generation system equipped with an additive supply system was fabricated and tested for the performance evaluation experimentally and analytically, in order to confirm the advantage of *in situ* oxidation-resistant coatings on gas turbine components toward the performance of a gas turbine power generation system directly. The gas turbine was operated up to the rated speed of 74,000 rpm, and to the turbine inlet temperature (TIT) of $\sim$1200 °C. At the early stage of this test operation, an oxide film precursor (tetraethylorthosilicate/methanol mixture, 10 vol.%) was fed into the combustion chamber by the additive supply system to *in situ* deposit silica based layers and thus to protect the metallic components from hot combustion gas during operation. After the test operation, *in situ* deposited silica layers were observed on the surface of the combustion chamber, turbine nozzles and rotor blade. Due to these protective layers the gas turbine could be harmless tested at TIT = 950 °C, much higher than its design temperature of 850 °C. According to the performance analysis, a TIT increase of 100 °C was expected to be accompanied by $\sim$5% increase in the turbine rotation speed by consuming more fuel and air by 22% and 8%, respectively. As a result, the power output increased by 42% and the thermal efficiency from 12% to 14%. This result was well accorded with that of empirically obtained, indicating that no noticeable impacts on the performance due to *in situ* deposited layers on the components.

13/01000 Controlled autoignition of hydrogen in a direct-injection optical engine

Aleiferis, P. G. and Rosati, M. F. *Combustion and Flame*, 2012, 159, (7), 2500–2515.

Research into novel internal combustion engines requires consideration of the diversity in future fuels in an attempt to reduce drastically CO_2 emissions from vehicles and promote energy sustainability. Hydrogen has been proposed as a possible fuel for future internal combustion engines and can be produced from renewable sources. Hydrogen's wide flammability range allows higher engine efficiency than conventional fuels with both reduced toxic emissions and no CO_2 gases. Most previous work on hydrogen engines has focused on spark-ignition operation. The current paper presents results from an optical study of controlled autoignition (or homogeneous charge compression ignition) of hydrogen in an engine of latest spark-ignition pentroof combustion chamber geometry with direct injection of hydrogen (100 bar). This was achieved by a combination of inlet air preheating in the range 200–400 °C and residual gas recirculated internally by negative valve overlap. Hydrogen fuelling was set to various values of equivalence ratio, typically in the range $\phi = 0.40$–0.63. Crank-angle resolved flame chemiluminescence images were acquired for a series of consecutive cycles at 1000 rpm in order to calculate in-cylinder rates of flame expansion and motion. Planar laser-induced fluorescence of OH was also applied to record more detailed features of the autoignition pattern. Single and double (i.e. 'split' per cycle) hydrogen injection strategies were employed in order to identify the effect of mixture preparation on autoignition's timing and spatial development. An attempt was also made to review relevant in-cylinder phenomena from the limited literature on hydrogen-fuelled spark-ignition optical engines and make comparisons were appropriate.

13/01001 Effects of magnetic field on fuel consumption and exhaust emissions in two-stroke engine

Faris, A. S. *et al. Energy Procedia*, 2012, 18, 327–338.

The energy of permanent magnets was used in this research for the treatment of vehicle fuel (Iraqi gasoline), to reducing consumption, as well as reducing the emission of certain pollutants rates. The experiments in the current research comprised using permanent magnets with different intensities (2000, 4000, 6000 and 9000 gauss), which were installed on the fuel line of a two-stroke engine. The authors studied the impacts on gasoline consumption, as well as exhaust gases. It was necessary to search for experiments without the use of magnets for comparison purposes. The overall performance and exhaust emission tests showed a good result, where the rate of reduction in gasoline consumption ranges from 9 to 14%. The larger reduction value of 14% was obtained using a field intensity of 6000 gauss as well as the intensity 9000 gauss. It was found that the percentages of exhaust gas components (CO, HC) were decreased by 30% and 40%, respectively, but CO_2 percentage increased up to 10%. Absorption spectrum of infrared and ultraviolet radiation showed a change in physical and chemical properties in the structure of gasoline molecules under the influence of the magnetic field. Surface tension of gasoline exposed to different intensities of magnetic field was measured and compared with these without magnetization.

13/01002 Measurement of in-cylinder soot particles and their distribution in an optical HSDI diesel engine using time resolved laser induced incandescence (TR-LII)

Menkiel, B. *et al. Combustion and Flame*, 2012, 159, (9), 2985–2998.

Soot particles generated during combustion process in a single cylinder optical diesel engine were measured using time-resolved laser induced incandescence technique (TR-LII). Experimentally measured LII data were fitted with theoretically simulated LII data to determine the count median particle diameter and the geometric width of the particle size distribution. TR-LII signals were acquired simultaneously at two different wavelengths for crank angles in the range from 48.4° to 111.4° after top dead centre (aTDC) and for various engine operating conditions. Particle size was found to be dependent on the engine load but no significant change in particle sizes were observed for different fuel injection timings. The average size of the primary particles measured over different crank angles were larger at higher engine loads compared to lower engine loads. A general trend of the soot particle diameter decreasing with crank angle was observed due to oxidation, but towards the end of the expansion stroke a marginal increase in size was noted. For all operating conditions the width of the particle size distribution was found to decrease with crank angle until 61.4° aTDC, and thereafter it increases to reach a well-defined size distribution for a given fuel injection quantity despite the differences in the injection timing. The soot particles are randomly transported by the complex fluid motion present within the combustion chamber leading to strong cycle to cycle fluctuations of the measured time resolved LII data. The in-cylinder soot volume fraction derived from TR-LII data revealed that for different fuel injection timings, a relatively higher amount of soot was produced for shorter ignition delay compared to larger ignition delays.

13/01003 Numerical analyses of EGR techniques in a turbocharged spark-ignition engine

Galloni, E. *et al. Applied Thermal Engineering*, 2012, 39, 95–104.

Exhaust gas recycle (EGR) is an interesting technique, which is more and more adopted in spark-ignition engines in order to reduce both NO_x emissions and fuel consumption in certain engine operating points. A fraction of exhaust gases recycled to the intake produces a significant charge dilution which decreases the combustion chamber temperature and, as a consequence, the NO formation rates. Furthermore, charge dilution allows reducing pumping losses at part load and heat losses through the walls increasing the engine efficiency. In this paper, numerous numerical analyses have been carried out in order to widely estimate the potential of exhaust gas recycle in a downsized, turbocharged spark-ignition engine. Many engine operating points have been examined, at different speed and load. Major attention has been paid to the portion of the engine map characterized by low rotational speed and WOT operation. Thus, the most severe conditions for knock onset have been deeply investigated. The combustion process has been modelled by means of a three-dimensional computational code. In particular, an in-cylinder analysis has been carried out to evaluate the effects of charge dilution on flame propagation, knock resistance and exhaust gas temperature distribution. Furthermore, adopting EGR, main engine control parameters (fuel to air ratio, spark advance and boost pressure) have been recalculated and the overall performances have been computed by a one-dimensional model. In this case, a simplified combustion model, tuned by means of three-dimensional computations, has been utilized. The models here presented have been validated by several comparisons with experimentally obtained results. The optimization of engine parameters, together with the evaluation of knock risks, allowed recovering, at some extent, the engine performance in absence of exhaust recycle. At the same time, reductions in both fuel consumption and pollutant emissions have been obtained.

13/01004 Online estimation of turbine–generator shaft fatigue loss-of-life caused by subsynchronous resonance

Xie, X. *et al. Electric Power Systems Research*, 2012, 92, 171–179.

In this paper, a novel approach is presented to estimate the fatigue loss-of-life (FLoL) of larger turbine–generators that suffer from subsynchronous resonance (SSR) in series-compensated power systems. The most important contribution of the proposed approach is to estimate the mechanical torques of the turbine–generator shaft in real time with the terminal speed of the shaft and the voltage/current of the generator. With the estimated torques and the manufacturer-provided stress/torque-versus-life or S/T–N curves, FLoL can be obtained online by the well-known rainflow cycle counting technique. This approach is embedded in SSR protective or monitoring system to supervise possible FLoL due to system disturbances. As a case study, it was implemented in the torsional stress relay or TSR for the generator of the Shangdu power plant, which was threatened by SSR problem caused by fixed capacitor compensation. The response of the TSR during an actual fault of the studied system was recorded. Electromagnetic simulation was conducted for this specific fault. The torques and FLoL were estimated as well as compared with theoretical values and recorded data. The results showed a very good consistency and thus verified the effectiveness of the proposed approach.

13/01005 The effect of fuel pretreatment on performance of pulse detonation rocket engines

Fan, Z. C. *et al. Experimental Thermal and Fluid Science*, 2012, 41, 130–142.

For hypersonic potential-use pulse detonation rocket engines (PDREs), the detonation chamber must stand against the high intensity of waste heat by fuel active cooling which in turn preheats and promotes liquid hydrocarbon fuel to crack into lower-molecular-weight carbon alkenes. The purpose of this research was to study the beneficial effects of the fuel pretreatments on PDRE performance, which comprised preheating and adding additives. Firstly, five concentric-counter-flow heat exchangers based on active cooling were tested to investigate the effect of geometric dimension on the heating efficiency. The results showed that the optimum length and thickness of annular heat exchange section were 300 and 5 mm, respectively. The heating capacity of the heat exchanger based on active cooling was significant. Furthermore, the effects of heat exchanger on operation time duration of PDRE and atomization improving of liquid kerosene were then investigated. The results indicated that the operation time of PDRE were extended nearly three times and PDRE could be operated normally without fuel injector. The initiation time was a very important factor for the multi-cycle PDRE, which was the sum of ignition delay time and whole deflagration-to-detonation transition run-up time; therefore, experiments were conducted to investigate the effects of the fuel preheating and adding additives on the detonation initiation time. The results demonstrated that with the aid of fuel preheating, the detonation initiation time for liquid kerosene was noticeably reduced and the operation time of PDRE was remarkably prolonged, a fully-developed detonation wave was achieved in the position away from igniter 8.33 times of the diameter of the detonation tube. By adding the additives to liquid kerosene, the detonation initiation time from 0.75 ms decreased to 0.34 ms and the detonability of fuel was dramatically improved.

Hybrid engine systems

13/01006 Cold start characteristics of an ethanol-fuelled engine with heated intake air and fuel

Sales, L. C. M. and Sodré, J. R. *Applied Thermal Engineering*, 2012, 40, 198–201.

The conventional cold start system of flexible fuel engines introduces gasoline in the intake system when the vehicle is fuelled with hydrous ethanol or with high ethanol content gasoline–ethanol blends. The system is necessary to allow for ignition of the fuel–air mixture under low temperatures due to the high ethanol evaporation temperature, in comparison with gasoline. This works presents a new cold start system for flexible fuel engines with heating of intake air and ethanol injector. The removal of the gasoline reservoir for cold start is the main benefit of the new system, and it is an awaited evolution of flexible fuel engines. The experimental results demonstrate that the new system provides hydrous ethanol-fuelled engine start in less than 2 s under temperatures as low as 0 °C.

13/01007 Combustion behaviour of a heavy duty common rail marine diesel engine fumigated with propane

Goldsworthy, L. *Experimental Thermal and Fluid Science*, 2012, 42, 93–106.

This paper presents results from the testing of a heavy duty common rail marine diesel engine with electronically controlled two stage liquid fuel injection, operating under load on a test bench with propane mixed into the inlet air at various rates. Results are presented for a range of engine loads, with brake mean effective pressure up to 22 bar at 1800 rpm. The electronic engine control unit is not modified and allowed to respond to the addition of propane according to its inbuilt map. This results in retarded injection timing with increased propane addition at some test points. At each test point, constant engine speed and brake torque are maintained for various rates of propane addition. Cylinder pressure and the injector activation voltage are recorded with a high speed data acquisition system. Apparent heat release rate is calculated from the measured cylinder pressure. At high rates of propane addition very high pressure rise rates and severe knock are measured. At the high brake mean effective pressure conditions tested, knock limits propane supply rates to less than 20% by energy. Small increases in thermal efficiency are indicated with moderate rates of propane addition. Exhaust emissions of NO_x, CO, HC and smoke are measured. CO, HC and smoke emissions increase significantly with increasing propane addition. For high propane supply rates, two distinct peaks in heat release rate are measured. Analysis is made of the flammability of the propane–air mixtures at the elevated temperatures at the end of the compression stroke, using the modified Burgess–Wheeler law. At propane supply rates greater than 25%, the propane–air mixture is flammable in its own right at compression temperature. The apparent heat release rate, fuel injection timing and flammability data allow analysis of the mechanism of the combustion process with propane fumigation.

13/01008 Efficiency and emissions in a vehicle spark ignition engine fueled with hydrogen and methane blends

Moreno, F. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11495–11503.

This paper shows the results of the tests carried out in a naturally aspirated vehicle spark ignition engine fuelled with different hydrogen and methane blends. The percentage of hydrogen tested was up to 50% by volume in methane. The tests were carried out in a wide range of speeds with the original ignition timing of the engine. Also, lean equivalence ratios were proved. Just the fuel injection map was modified for each fuel blend and equivalence ratio tested. In this paper, the results of thermal efficiency and pollutant emissions achieved at full load have been compared with the corresponding gasoline test results. The best balance between thermal efficiency and pollutant emissions was observed with the 30% hydrogen and 70% methane fuel blend.

13/01009 On-road performance comparison of two identical cars consuming petrodiesel and biodiesel

Serrano, L. *et al. Fuel Processing Technology*, 2012, 103, 125–133.

This work studies the impact on vehicle performance and fuel consumption when using 100% diesel with petroleum origin (fossil diesel), compared to a mixture of 20% biodiesel in 80% of fossil diesel fuel (B20). For the accomplishment of this work an assessment was made using some primary tests on a chassis dynamometer, measuring vehicle performance and consumption. Subsequently a methodology was developed to conduct road tests. These considered the simultaneous circulation of two identical vehicles, fed with the two different fuels, but running on the same traffic and road conditions. Both vehicles were equipped with geo-referencing systems and data measured by the electronic control unit were acquired. A precision balance was used in fuel consumption measurements of an auxiliary reservoir. The results demonstrate that the use of biodiesel has a penalizing effect on the mass fuel consumption and on vehicle's performance, but this is largely dependent on the type of circuit used. One can also conclude that the methodology implemented on the study of fuel alternatives is extremely important. It is noticeable that for different route needs, different energetic solutions are more suitable than others, which can only be properly assessed by conducting road tests.

Transport battery development

13/01010 Analysis of a scenario of large scale adoption of electrical vehicles in Nord-trøndelag

Vatne, Å *et al. Energy Procedia*, 2012, 20, 291–300.

The purpose of this paper was to show the strain on the grid by implementing a large share of electrical vehicles (EVs). The result from the manually simulations shows that the system in not capable of handling a dumb-charging approach when the share of EVs are 63%, while the simulations from PSCAD show that the voltage limits are not exceeded. The lowest measured voltage in the dumb charging is measured to 0.984 p.u. This is a voltage drop of 1.6% and therefore does not exceed the limits of ±10%. It was expected that the voltage drop in the dumb charging approach would be larger. The sources of error have not yet been located. The trend of the results does however show that a smart charge approach will cause less strain on the grid. A large-scale adoption of EVs is an intelligent way to reach this goal and addition have a more efficient usage of the available power, and especially in a network with a high share of renewable resources. The result from the analysis shows that the smart charging approach did not causes any extra strain on the demand during the peak hours. A large share adoption of EVs requires beneficial infrastructure. In addition to slow charging from a suitable docking station (mode 2/mode 3), fast chargers (mode 4) need to be included in the infrastructure. Mode 1, which is the most used charging mode today, will fade out and be replaced. The chargers at residents and workplaces will mainly consist of mode 2 and mode 3 chargers. To be able to introduce the vehicle to home (V2H) solution, the charging technologies need to be based on mode 3 charging described in IEC 61851–1. Mode 3 requires control and signal pins for both the charger side and the vehicle side. An introduction of V2H and generally smart charging forward a huge opportunity for a third-party to offer add-ons and other business ideas.

13/01011 Chemical-free synthesis of graphene–carbon nanotube hybrid materials for reversible lithium storage in lithium-ion batteries

Chen, S. *et al. Carbon*, 2012, 50, (12), 4557–4565.

Graphene–carbon nanotube hybrid materials were successfully prepared through the π–π interaction without using any chemical reagent. The authors found that the ratio between carbon nanotube and graphene had critical influences on the state in aqueous solution and morphology of hybrid materials. Field emission scanning electron microscope and transmission electron microscope analysis confirmed that graphene nanosheets wrap around individual carbon nanotubes and form a homogeneous three-dimensional hybrid nanostructure. When applied as an anode material in lithium ion batteries, graphene–carbon nanotube hybrid materials demonstrated a high reversible lithium storage capacity, a high Coulombic efficiency and an excellent cyclability.

13/01012 Day-ahead tariffs for the alleviation of distribution grid congestion from electric vehicles

O'Connell, N. *et al. Electric Power Systems Research*, 2012, 92, 106–114.

An economically efficient day-ahead tariff (DT) is proposed with the purpose of preventing distribution grid congestion resulting from electric vehicle (EV) charging scheduled on a day-ahead basis. The DT concept developed herein is derived from the locational marginal price (LMP), in particular the congestion cost component of the LMP. A step-wise congestion management structure has been developed whereby the distribution system operator (DSO) predicts congestion for the coming day and publishes DTs prior to the clearing of the day-ahead market. EV fleet operators (FOs) optimize their EV charging schedules with respect to the predicted day-ahead prices and the published DTs, thereby avoiding congestion while still minimizing the charging cost. A Danish 400 V distribution network is used to conduct case studies to illustrate the effectiveness of the developed concept for the prevention of distribution grid congestion from EV charging. The case study results show that the concept is successful in a number of situations, most notably a predicted system overload of 155% can be successfully alleviated on the test distribution network.

13/01013 Design and control of a PEMFC powered electric wheelchair

Wang, F. C. and Chiang, Y. S. *International Journal of Hydrogen Energy*, 2012, 37, (15), 11299–11307.

This paper proposes the design and control of a fuel-cell powered wheelchair. Electric wheelchairs can improve moving ability for people with walking problems. However, their travelling distances are limited by the capacity of their batteries. The authors designed a fuel-cell powered electric wheelchair that can be continuously operated, thereby extending the moving range. The system consisted of three subsystems: a commercial electric wheelchair, a proton exchange membrane fuel cell (PEMFC), and two secondary battery sets. The study was carried out in three parts, investigating the fuel-cell control, power management, and system integration. First, they designed multivariable robust controllers for a 500 W PEMFC system to charge the battery sets by constant voltage/current. Second, they designed a serial power management system, where the wheelchair motors were directly driven by the secondary battery sets, which in turn were charged by the PEMFC when their capacities dropped below a certain level. Lastly, the authors integrated the three subsystems and verified the system performance by experiments. The results confirmed the effectiveness of the PEMFC system as a way to extend the travelling distance of a motorized wheelchair.

13/01014 Double resonant isolated converter for battery charger with fast switching semiconductors used in hybrid electric shunting locomotive

Bernardinis, A. D. *et al. Electric Power Systems Research*, 2012, 92, 43–49.

This paper presents the study and experimental validation of a 9 kW lead-acid battery charger used to feed the 72 V DC-Bus inside a hybrid electric locomotive demonstrator realized in the frame of the French research project PLATHEE (energy-efficient and environmentally friendly train platform). The role of the converter is to supply the 72 V DC consumers and charge the battery. The proposed topology for the battery charger is a DC/AC/DC step-down converter structure using high frequency transformer and double resonant series-parallel dipole. Main advantages of this topology are losses minimization due to soft switching operation, reduction of passive component weight and easy system integration. However, development and testing of the converter remain complex owing to high frequency constraints. Anti-parallel diodes of DC/AC half-bridge dissipate losses in excess during switching sequences and their reverse recovery energy leads to constraining high current peaks. A solution consists in using fast insulated gate bipolar transistor (IGBT)/diode technology well suited to high frequency switching, and able to limit diode peak-current amplitude during switch-off. Electro-thermal endurance tests have been performed in order to characterize the thermal behaviour of the semiconductor module and control its case temperature raising. The battery charger working has been first validated on laboratory test-bench using a battery emulator, and then implemented in the hybrid locomotive for electrical couplings tests.

13/01015 GHGT-9 phosphate materials for lithium batteries and energy storage

Gauthier, M. *Procedia Engineering*, 2012, 46, 234–254.

The trend to electrification in society calls for other sources of energy and storage than carbon materials, especially fossil ones. Lithium batteries have emerged in the last decades as a convenient way to store and deliver the most noble and versatile form of energy: electricity. From cell phones and other portable applications, the technology is now growing fast as a vector to store energy for transportation and use on the grid. Lithium's light weight, its reactivity to form Li_2O and its small ionic radius have led to the development of Li-insertion oxide structures that can act as electrode materials or electrolytes. Phosphate materials have recently been discovered that can make new stable complex oxide structures allowing the design of safer, performing and economically viable large-scale storage batteries, C-LiFePO4 being the most successful one to date.

13/01016 Greenhouse gas emissions of electric vehicles associated with wind and photovoltaic electricity

Querini, F. *et al. Energy Procedia*, 2012, 20, 391–401.

Until recently, the automotive industry was solely relying on one energy resource: oil. However, because of several environmental, political and economic issues, new alternatives are now emerging, such as electric vehicles (EVs). The greenhouse gas (GHG) emissions of an EV are linked with the manufacturing of the car and the electricity production during the use phase. This paper studies the GHG emissions linked with EVs using photovoltaic (PV) and wind electricity associated with a Renault EV. GHG emissions are compared with EVs using average electricity from various European countries and from conventional thermal vehicles. The results show that using wind electricity always allows decreasing GHG emissions while PV impact is dependent on the country studied. Nonetheless, when using PV electricity, GHG emissions are always lower than conventional thermal vehicles.

13/01017 Ordered mesoporous carbon–TiO_2 materials for improved electrochemical performance of lithium ion battery

Chang, P. Y. *et al. Carbon*, 2012, 50, (11), 4259–4268.

A series of ordered mesoporous carbon–TiO_2 (OMCT) materials with various weight percentages of TiO_2 (50–75 wt%) were synthesized by evaporation-induced self-assembly and *in situ* crystallization at various calcination temperatures (600–1200 °C) to evaluate the Li-ion storage performance. The OMCT has ordered two-dimensional hexagonal mesoporous structures and the TiO_2 nanocrystals with different phases are embedded into the frameworks of carbonaceous matrix. The reversible capacity of OMCT is highly dependent on the phase and content of TiO_2, and the anatase TiO_2 is a superior crystalline phase to rutile and TiN for Li-ion insertion. The $OMCT_{65}$ which contains 35 wt% carbon and 65 wt% TiO_2 shows a high capacity of 500 mAh g^{-1} at 0.1C after 80 cycles. In addition, $OMCT_{65}$ exhibits a good cyclability and rate capability. The reversible capacity remains at 98 mAh g^{-1} at a high rate of 5C, and then recoveries to 520 mAh g^{-1} at 0.1C after 105 cycles. The excellent reversible capacity and rate capability of $OMCT_{65}$ are attributed to the embedment of well-dispersed anatase TiO_2 nanocrystals into the specific porous structure of OMCT, which can not only facilitate the fast Li-ion charge transport but can also strengthen the carbon–TiO_2 co-constructing channels for lithiated reactions.

12 REFRACTORIES/ CERAMICS

Properties, production, applications

13/01018 A low-cost counter electrode of ITO glass coated with a graphene/Nafion® composite film for use in dye-sensitized solar cells

Yeh, M. H. *et al. Carbon*, 2012, 50, (11), 4192–4202.

Carbon black (CB), multi-walled carbon nanotube (MWCNT), and graphene (GN) were examined as catalytic films on the counter electrodes (CEs) of dye-sensitized solar cells (DSSCs). GN exhibits the best performance among these materials for the corresponding cell. A composite film of GN/Nafion® was next used as the catalytic film on the CE of a DSSC. Nafion® is demonstrated to be an excellent dispersant for inhibiting the aggregation of GN. A solar-to-electricity conversion efficiency (η) of 8.19% was achieved for the DSSC sensitized by TBA(Ru[(4-carboxylic acid-4′-carboxylate-2,2′-bipyridine)(4,4′-bis(5-(hexylthio)-2,2′-bithien-5′-yl)-2,2′-bipyridine)($NCS)_2$]), i.e. CYC-B11 dye, which was synthesized by this group, after the optimization of the composition of GN/Nafion®, and an η of 8.89% was exhibited for the cell with a sputtered-Pt (s-Pt) film on its CE under the same conditions. The significance of the cell with the composite film of GN/Nafion® lies in the fact that the expensive Pt is avoided in this case, thereby the cost of the pertinent DSSC was greatly reduced, even though its η (8.19%) is slightly smaller than that of the cell with the s-Pt film (8.89%).

13/01019 A new formulation of barium–strontium silicate glasses and glass-ceramics for high-temperature sealant

Sharma, K. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11360–11369.

P_2O_5 is a common nucleating agent in glass-ceramics. To avoid the negative effect of P_2O_5 on sealing glass properties, the authors combined it with barium oxide in the glass formulation. The effect of $Ba_3(PO_4)_2$ incorporation on thermophysical, structural and sealing characteristics of a glass of composition (mol%) $30SiO_2$–20SrO–30BaO–$10B_2O_3$–$5La_2O_3$–$5Al_2O_3$ is reported. The glass transition temperature decreases from 650 °C to 584 °C when $Ba_3(PO_4)_2$ is increased from 0 to 2 mol%. Thermal expansion coefficient of the glass samples are found around 11.4 to $12.0 \times 10^{-6}\,°C^{-1}$, which is close to that of Crofer-22 APU. ^{29}Si MAS-NMR measurements indicate that glass network is composed of mainly Q^2 units, while ^{31}P forms Q^0 units. XRD shows the formation of Ba_2SiO_4, Sr_2SiO_4 and $BaAl_2Si_2O_8$ crystalline phases. There is no further evolution of crystalline phases when heat treated at 800 °C for 500 h. Seals with Crofer-22 plates have been made and interface reveals good bonding. The glass composition formulated by addition of 1 mol% $Ba_3(PO_4)_2$ has shown good thermal and sealing characteristics, while further increase of $Ba_3(PO_4)_2$ to 2 mol% leads to increased crystallization tendency.

13/01020 Clay interaction with liquid and supercritical CO_2: the relevance of electrical and capillary forces

Espinoza, D. N. and Santamarina, J. C. *International Journal of Greenhouse Gas Control*, 2012, 10, 351–362.

Caprocks with significant clay content are candidate seal layers for CO_2 geological storage. Changes in electrical and capillary forces are expected when CO_2 invades the water saturated pore space. Sedimentation experiments conducted to explore the response of kaolinite and montmorillonite to deionized water, brine, heptane, liquid CO_2 and supercritical CO_2 show that both montmorillonite and kaolinite aggregate when submerged in CO_2 and the final porosity in CO_2 is smaller than in brine. Differences in dielectric properties between CO_2 and water, and ensuing implications on van der Waals attraction and double layer repulsion explain the observed phenomena. On the other hand, capillary effects induced by the water–CO_2 interface are corroborated by clay–water paste desiccation experiments conducted using supercritical CO_2: water dissolution into the surrounding CO_2 causes suction and capillary contraction, the invasion of the CO_2–water interface into the sediment, and the formation of desiccation cracks. Volume contraction and crack initiation are consistent with the sediment response within an effective stress framework. Altered electrical forces and emergent capillary forces lead to coupled chemo-hydro-mechanical phenomena in seal layers that could facilitate CO_2 breakthrough and advection through high porosity caprocks; related phenomena are identified in the reservoir rock. Additional studies are needed to further assess coupled phenomena when the interparticle distance is a few monolayers of water.

13/01021 Coupling effects of foam ceramics on the flame and shock wave of gas explosion

Zhang, J. *et al. Safety Science*, 2012, 50, (4), 797–800.

The coupling of gas explosion flame and shock wave is analysed. In the gas explosion process, shock wave is affected by the flame directly, and shock wave also induces the flame. Inhibiting explosion can be achieved by the interference between the flame and shock wave propagation. If the coupling effects can be damaged, the adverse effects caused by the explosion should be mitigated and controlled. According to the structure characteristics of foam ceramics, the coupling effects mechanism of ceramic foam on gas explosion flame and shock wave is researched. When the explosion goes through the structure of foam ceramics, the flame can be quenched and the shock wave be attenuated. After the flame is quenched, the supply of precursor shock wave energy is cut off. Due to lack of energy supply, the destructive effects of blast wave will be reduced effectively. Coupling effects of the flame and shock wave can be damaged by the special structure of foam ceramics. Studies suggest that a certain function to represent the structure characteristics of foam ceramics must exist. For a certain material of foam ceramics, the sure porosity δ and the pore diameter d also can be get, which is the key to research and develop foam ceramic suppression technology of gas explosion.

13/01022 Effective atomic numbers for some calcium–strontium-borate glasses

Sharma, R. *et al. Annals of Nuclear Energy*, 2012, 45, 144–149.

Effective atomic number acts as a fundamental property of compounds and mixtures and also plays a key role in the computation of various dosimetric parameters such as build-up factor, effective dose and heat generation. Effective atomic numbers have been computed in the energy range from 1 keV to 100 GeV for different chemical compositions of calcium–strontium-borate glasses. The effective atomic number values have been computed and compared by two different methods: (a) ratio of atomic to electron cross-section and (b) logarithmic interpolation of molecular cross-section values. It has been observed that in the lower energy region, two interpolation regions occur for all the selected glasses, which results in two effective number values at the same energy. Hence, experimental verification of effective atomic number is required in the lower energy region.

13/01023 Effects of glazing colour type on perception of daylight quality, arousal, and switch-on patterns of electric light in office rooms

Arsenault, H. *et al. Building and Environment*, 2012, 56, 223–231.

A study is presented about the effects of three glazing colour types (blue, neutral, bronze) on daylight quality, arousal and switch-on patterns for electric lights. This study was carried out using a scale model (1:4) of an office room, where subjective evaluations of the luminous conditions were performed by 36 participants (mean age 23.8 years) with their upper bodies immersed in the model. The evaluations were achieved using questionnaires designed to assess five light quality factors: (1) visual comfort; (2) naturality; (3) pleasantness; (4) precision (of details and textures) and (5) light level. Mixed model analyses of the questions revealed significant higher scores for pleasantness ($p = 0.003$) comfort ($p = 0.015$) and light level ($p = 0.044$) for the bronze glazing type compared to the blue and neutral glazing, confirming results of earlier studies. Results from a paired *t*-test on the Karolinska sleepiness scale scores indicated that the level of self-reported arousal decreased in presence of the blue glazing. However, the analysis did not reveal significant results regarding switch-on patterns of electric lights. Overall, the study shows that there is a preference for daylight filtered through bronze window glazing and that the glazing colour type may have a significant effect on arousal level of office workers.

13/01024 Fischer–Tropsch synthesis over cobalt based catalyst supported on different mesoporous silica

Jung, J. S. *et al. Catalysis Today*, 2012, 185, (1), 168–174.

Fischer–Tropsch synthesis (FTS) has been suggested as a key process of gas-to-liquid (GTL) technology, to satisfy the increasing demands for high-quality and environmentally friendly fuels. In this work, the catalytic performance of cobalt catalyst supported on various periodic mesoporous silicas was investigated. Silica modified Co-based catalysts were prepared by a sol–gel method followed by an impregnation method. The characteristics of supports and of the catalysts were identified by N_2 physisorption, CO chemisorption, TPR, XPS, XRD, SEM/EDX and TEM techniques. Their catalytic performance for FTS was evaluated in a fixed-bed reactor with H_2/CO molar ratio of 2, reaction temperature of 230 °C and reaction pressure of 20 bar. The Co/SHS catalyst supported on periodic mesoporous silica hollow sphere shows higher catalytic performance and C_5^+ selectivity in FTS reaction than the other catalysts. It was considered that catalytic performance of cobalt based catalysts supported on various silica in FTS depends on the cobalt particle size and support structure, which is caused by pore diameter and pore size distribution.

13/01025 Microcrystalline silicon carbide window layers in thin film silicon solar cells

Chen, T. *et al. Solar Energy Materials and Solar Cells*, 2012, 98, 370–378.

Crystalline silicon carbide alloys have a very high potential to be used as transparent conductive window layers in thin-film solar cells provided they can be prepared in thin-film form and at compatible deposition temperatures. Using hot-wire chemical vapour deposition (HWCVD) technique, silicon carbide in microcrystalline form (μc-SiC:H) has been prepared at low substrate temperature. Monomethylsilane and hydrogen are used as the precursor gases. The material is highly conductive, unintentionally n-type in nature, and possess wide optical gap. These properties have been utilized by employing the μc-SiC:H layer as the window layer in n-side illuminated single junction microcrystalline silicon (μc-Si:H) solar cells. Some typical issues related to this device research and development are described here. In particular the nucleation of the intrinsic μc-Si:H absorber layer on the n-type μc-SiC:H layer needs attention. With proper device design high short-circuit current densities of 29.6 mA/cm^2 and quantum efficiencies up to 90% are obtained resulting in a maximum conversion efficiency of 9.6% within a 2-μm-thick μc-Si:H solar cell.

13/01026 Numerical simulation on foam ceramic blasting block device under the action of explosion transform

Sun, J. *et al. Safety Science*, 2012, 50, (4), 588–592.

The responsive behaviour of the action of under explosion blasting block damaging device structure was investigated based on quality equation, energy conservation equation and thermodynamics equation, using the ANSYS finite element simulation and Euler form of momentum equation. This paper analysed the destructive situation of the inside and outside of the foam ceramic device. The research shows that the finite element simulation results and the numerical calculation results agree, which provides important reference basis in the anti-explosion design and improvement of cut off the device for blasting.

13/01027 Octalithium plumbate as breeding blanket ceramic: neutronic performances, synthesis and partial characterization

Colominas, S. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 482–485.

A neutronic assessment of the performances of a helium-cooled Li_8PbO_6 breeding blanket (BB) for the conceptual design of a DEMO fusion reactor is given. Different BB configurations have been considered in order to minimize the amount of beryllium required for neutron multiplication, including the use of graphite as reflector material. The calculated neutronic responses: tritium breeding ratio (TBR), power deposition in TF coils and power amplification factor, indicate the feasibility of Li_8PbO_6 as breeding material. Furthermore, the synthesis and characterization of Li_8PbO_6 by X-ray phase analysis are also discussed.

13/01028 On a multivariate population balance model to describe the structure and composition of silica nanoparticles

Shekar, S. *et al. Computers & Chemical Engineering*, 2012, 43, 130–147.

The aim of this work is to present the mathematical description of a detailed multivariate population balance model to describe the structure and composition of silica nanoparticles. A detailed numerical study of a stochastic particle algorithm for the solution of the multidimensional population balance model is presented. Each particle is described by its constituent primary particles and the connectivity between these primaries. Each primary in turn has internal variables that describe its chemical composition. The algorithms used to solve the population balance equations and to couple the population balance model to gas-phase chemistry are described. Numerical studies are then performed for a number of functionals calculated from the model to establish the convergence with respect to the numerical parameter that determines the number of computational particles in the system. The computational efficiency of the model is found to render it applicable to the simulation of industrial scale systems.

13/01029 On the experimental and numerical investigation of clay/epoxy nanocomposites

Silani, M. *et al. Composite Structures*, 2012, 94, (11), 3142–3148.

Due to increasing use of clay/epoxy nanocomposites in industry, investigation of mechanical properties of clay nanocomposites has become of great interest. While the stiffening mechanism of clay nanocomposites is well documented, there is still not a clear understanding about how the addition of clays affect the fracture behaviour of clay/epoxy nanocomposites. The main aim of this paper is to measure and explain the effect of clays on ductility reduction of these nanocomposites. First, epoxy and clay/epoxy nanocomposites with different clay weight ratio were built. Then, the damage parameters of epoxy and clay/epoxy nanocomposites were measured by variation of the elasticity modulus. Based on loading–unloading experiments, the Lemaitre damage parameters for epoxy and clay/epoxy nanocomposites were extracted. Crack initiation and propagation in dog-bone sample were simulated for epoxy and clay/epoxy nanocomposites using the extended finite element method (XFEM). The comparison between experimental and numerical results shows that the proposed method can predict the crack initiation location and propagation path in clay/epoxy nanocomposites.

13/01030 Oxidation of fuel cladding candidate materials in steam environments at high temperature and pressure

Cheng, T. *et al. Journal of Nuclear Materials*, 2012, 427, (1–3), 396–400.

Under certain severe accident conditions, the fuel rods of nuclear power plants are exposed to high temperature/pressure steam environments in which the Zr alloy cladding is rapidly oxidized. As alternative claddings, the oxidation resistances of SiC-based materials and stainless steels with high Cr and/or Al additions have been examined from 800–1200 °C in high-pressure steam environments. Very low reaction kinetics were observed with alumina-forming FeCrAl alloys at 1200 °C while Fe-Cr alloys with only 15–20% Cr were rapidly attacked.

13/01031 Performance of invertase immobilized on glass–ceramic supports in batch bioreactor

Albertini, A. V. P. *et al. Chemical Engineering Journal*, 2012, 187, 341–350.

Invertase was covalently immobilized on glass–ceramic support (GCS) obtained from coal fly ashes (CFA) with polyvinyl pyrrolidone (PVP) and magnesium stearate added as temporary additive. The GCS samples containing $Pb(CH_3COO)_2$, (GCS*Pb*) or $ZnSO_4$ (GCS*Zn*) were obtained in several sintering temperatures (1000–1200 °C) and times (1–3 h). The apparent values of porosity, water absorption, density and uniaxial compressive strength were studied by factorial design and morphological differences by scanning electron microscope. The best covalent immobilized invertase derivative was on GCS*Zn* (1200 °C/1 h) with 4398 ± 59.75 U/g GCS. However, 95.83% of immobilized invertase activity was obtained using an economical protocol with concentration of 0.636 mM 3-aminopropyltriethoxy silane (3-APTES) and 0.576 mM glutaraldehyde. The GCS*Zn*-invertase derivative retained 100% of initial activity after nine reuses (5476.19 ± 155.49 U/g GCS*Zn*). The CFA showed to be a promising biotechnological alternative as immobilization support for production of invert sugar and may be for other industrial enzymes.

13/01032 Phase composition and elemental partitioning in glass–ceramics containing high-Na/Al high level waste

Stefanovsky, S. V. *et al. Journal of Nuclear Materials*, 2012, 424, (1–3), 75–81.

Mixtures of surrogates of high level waste with high sodium and aluminium contents and sodium–lithium borosilicate frit were melted in alumina crucibles in a resistive furnace followed by quenching of one portion of the melt and annealing of the residual material in a turned-off furnace. The annealed materials with waste loading of up to 45 wt% contained minor spinel type phase and trace of nepheline $(Na,K)AlSiO_4$. In the annealed materials contained waste oxides in amount of 50 wt% and more nepheline and spinel were found to be major and minor phases, respectively. At high waste loadings two extra phases: Cs-aluminosilicate ($CsAlSiO_4$) and mixed Na/Cs-aluminosilicate were found in amount of 3–5 vol.% each. The latter phase contains of up to ~5.7 wt% SO_3 or 0.13 formula units S ($Na_{0.75}K_{0.05}Cs_{0.29}Ca_{0.02}Sr_{0.02}Al_{0.99}Fe_{0.03}Si_{0.76}S_{0.13}O_4$). Sulfur incorporation as S^{6+} or SO_4^{2-} ions into crystal lattice may be facilitated in the presence of large-size Cs^+ cations. Simplified suggested formula of this phase may be represented as $Na_{0.8}Cs_{0.3}AlSi_{0.8}S_{0.1}O_{3.95}$. It was also synthesized by sintering of mixture of chemicals at 1300 °C and found to be instable at temperatures higher than 1300 °C.

13/01033 Preparation and characterization of $BaCe_{0.95}Tb_{0.05}O_{3-\alpha}$ hollow fibre membranes for hydrogen permeation

Tan, X. *et al. Journal of the European Ceramic Society*, 2012, 32, (10), 2351–2357.

$BaCe_{0.95}Tb_{0.05}O_{3-\alpha}$ (BCTb) perovskite hollow fibre membranes were fabricated by spinning the slurry mixture containing 66.67 wt% BCTb powder, 6.67 wt% polyethersulfone (PESf) and 26.67 wt% N-methyl-2-pyrrolidone (NMP) followed by sintering at elevated temperatures. The influence of sintering temperature on the membrane properties was investigated in terms of crystal phase, morphology, porosity and mechanical strength. In order to obtain gas-tight hollow fibres with sufficient mechanical strength, the sintering temperature should be controlled between 1350 and 1450 °C. Hydrogen permeation through the BCTb hollow fibre membranes was carried out between 700 and 1000 °C using 50% H_2–He mixture as feed on the shell side and N_2 as sweep gas in the fibre lumen. The measured hydrogen permeation flux through the BCTb hollow fibre membranes reached up to $0.422\,\mu mol\,cm^{-2}\,s^{-1}$ at 1000 °C when the flow rates of the H_2–He feed and the nitrogen sweep were $40\,mL\,min^{-1}$ and $30\,mL\,min^{-1}$, respectively.

13/01034 Probabilistic lifetime prediction for ceramic components in rolling applications

Härtelt, M. *et al. Journal of the European Ceramic Society*, 2012, 32, (10), 2073–2085.

Rolling tools made of advanced ceramics have some attractive properties with respect to their wear resistance and high temperature performance but are critical due to the brittle failure mode. Lifetime predictions must be based on a probabilistic approach considering sub-critical and cyclic propagation of the inherent flaws. This study presents a comprehensive reliability analysis for a rolling contact fatigue test with a silicon nitride roll using the program STAU. Based on a cyclic crack growth law, the authors have extended the capabilities of STAU in order to account for a complex load history typically found in the case of rolling applications. A scheme is presented for relating the failure probability to the crack density observed on the roll which allows for a quantitative comparison of predictions and experimental observations. It turns out that the water-based lubrication most critically affects the failure behaviour since water strongly promotes cyclic crack propagation.

13/01035 Radiation damage of mesoporous silica thin films monitored by X-ray reflectivity and scanning electron microscopy

Dourdain, S. *et al. Journal of Nuclear Materials*, 2012, 427, (1–3), 411–414.

An innovative approach to investigate the effects of irradiation on mesoporous structure is proposed from the characterization of thin mesoporous silica films by X-ray reflectivity measurements coupled with scanning electron microscopy observations. Two different geometries of mesoporous thin films were irradiated with Xe ion beam. A collapse or a complete destruction of the porous structure depending on the pristine pore structure and an increase of the porosity attributed to track formation are discussed.

13/01036 Shielding and strength tests of silica fume concrete

Rezaei-Ochbelagh, D. *et al. Annals of Nuclear Energy*, 2012, 45, 150–154.

In this research, concrete containing different percentages of lead powder and silica fume was investigated as a gamma shield. Gamma photons emitted from gamma sources of ^{137}Cs and ^{60}Co were passed through concrete specimens and detected by two inches NaI(Tl) detector to investigate the attenuation coefficients of the specimens. Next, the compressive strengths of the specimens were experimentally studied. A comparison of concrete with and without silica fume revealed that although the addition of silica fume results in a slight reduction of the attenuation coefficient, which is negligible, it increases the compressive strength of concrete significantly. The results suggest the usefulness of 15% silica fume in concrete containing lead as a gamma shield.

13/01037 Study of ceramic pebble beds in post irradiation examination of the pebble bed assemblies irradiation experiment

Til, S. v. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 885–889.

The irradiation experiment pebble bed assemblies (PBA) consists of four mock-up representations (test elements) of the European Union helium cooled pebble bed (HCPB) concept. The four test elements contain a ceramic breeder pebble bed sandwiched between two beryllium pebble beds and are regarded as one of the first DEMO representative HCPB blanket irradiation tests, with respect to temperatures and power densities. The design value of the PBA were to irradiate pebble beds at a power density of 20–26 W/cc in the ceramic breeder, to a maximum temperature of 800 °C. Two test elements contain lithium orthosilicate pebbles (Li_4SiO_4; FZK/KIT) and were irradiated with target temperatures of 600 and 800 °C, respectively. The other test elements have lithium metatitanate (Li_2TiO_3; CEA) with different grain sizes and were both irradiated with a target temperature of 800 °C. The PBA have been irradiated for 294 full power days (12 cycles) in the high flux reactor (HFR) in Petten to a total neutron dose of 2–3 dpa in Eurofer, and an estimated (total) lithium burnup of 2–3% in the ceramic pebbles. This work presents results of post irradiation examinations (PIE) on the four HCPB test elements. Using for example SEM, the evolution of compressed pebble beds and pebble interactions like swelling, creep, sintering, etc., under irradiation and thermal loads are studied for the candidate pebble materials Li_2TiO_3 and Li_4SiO_4. (Chemical) interactions between ceramic pebbles and Eurofer (e.g. chrome diffusion) are observed. Looking at different sections of the pebble beds, correlations between temperatures and thermal–mechanical behaviour are clearly observed.

13/01038 The dual effect of Mg on the long-term alteration rate of AVM nuclear waste glasses

Thien, B. M. J. *et al. Journal of Nuclear Materials*, 2012, 427, (1–3), 297–310.

Inactive Mg-containing nuclear waste glasses simulating actual HLW glasses produced at the AVM facility since 1995 (Marcoule, France), were leached in aqueous solution in order to assess their long term behaviour. The focus was on the effect of Mg. The findings show that the distribution of Mg between the gel and the secondary crystalline phases strongly influences the glass dissolution rate. The glasses were leached in initially pure water ($T = 50$ °C, surface/volume ratio $(S/V) = 55\,cm^{-1}$) with and without addition of Mg^{2+} in the solution. ‘Mg-free’ AVM glasses were also leached in initially pure water (50 °C, $200\,cm^{-1}$) with and without addition of Mg^{2+} in the solution. Accurate identification of Mg-smectite secondary phases and gel composition calculations enable us to explain the different observed behaviours. Glass AVM 10 was the less altered glass in pure water. Its gel is more protective than the other probably because it is mainly balanced by Mg^{2+}. The addition of Mg^{2+} in the solution triggers the precipitation of smectite (not observed in pure water experiments), which consumes silicon from the gel, leading finally to a significant increase of the glass alteration. The authors also focused on the AVM 6 glass which was the most altered glass in pure water of available AVM glasses. Contrary to AVM 10, the gel of AVM 6 is mainly balanced by Na^+. The addition of Mg^{2+} in the solution allows the replacement of Na by Mg within the gel. This reaction clearly improves the gel properties and allows the rate to decrease more rapidly, in spite of the precipitation of smectite (also observed in pure water experiments). Finally, the two glasses were altered in synthetic groundwater (SGW) with a high Mg–Ca content. As expected from the previous observations, AVM 10 was insensitive to the presence of alkaline earths in the leaching solution whereas AVM 6 glass exhibited a lower rate than in pure water thanks to the incorporation of Mg and Ca within the gel.

13/01039 The use of lightweight expanded clay aggregate (LECA) as sorbent for PAHs removal from water

Nkansah, M. A. *et al. Journal of Hazardous Materials*, 2012, 217–218, 360–365.

Lightweight expanded clay aggregate (LECA) has been explored as a sorbent for the removal of PAHs (phenanthrene, fluoranthene and pyrene) from water. The efficacy of LECA as a sorbent for PAHs was assessed using contact time, mass of sorbent and sorption isotherms in a series of batch experiments. Maximum (optimum) sorption was reached at 21 h after which the amount of PAHs sorbed remained almost constant. Batch experiments were conducted by shaking a 100 ml solution mixture of individual PAHs (containing 0.02 mg/L) with LECA. The maximum sorption was 70.70, 70.82 and 72.12%, respectively for phenanthrene, fluoranthene and pyrene when a mass of 0.2 g of sorbent was used. There was an increase in sorption as a result of an increase in mass of sorbent until a maximum was reached at a mass of 4.0 g LECA with 92.61, 93.91 and 94.15% sorption of phenanthrene, fluoranthene and pyrene respectively. Sorption data were fitted to the linearized forms of the Freundlich and Langmuir isotherm models to determine the water-LECA partitioning coefficient. Physical sorption caused by the aromatic nature of the compounds was the main mechanism that governed the removal process while the hydrophobicity of the PAHs also influenced the sorption capacity. LECA can be used as an alternative method for aqueous PAHs removal.

13/01040 Thermal conductivity and heat transfer of ceramic nanofluids

Buschmann, M. H. *International Journal of Thermal Sciences*, 2012, 62, 19–28.

This study is motivated by the controversies surrounding nanofluids. Employing a rather simple but well-defined test rig it is shown that heat transfer can be enhanced by nanofluids in the thermal entrance region of laminar pipe flow. The thermophysical properties necessary to interpret the results of these experiments are measured very carefully. It is found that the thermal conductivity of five different ceramic nanofluids – measured with a sophisticated ring gap apparatus – do not show any anomalous behaviour. However, the dynamic viscosity is significantly increased compared with the basefluid.

13/01041 Valorization of biodiesel production residues in making porous clay brick

Eliche-Quesada, D. *et al. Fuel Processing Technology*, 2012, 103, 166–173.

In this study, the use of waste produced in biodiesel production plants, as spent earth from biodiesel filtration and the by-product of glycerine, in producing lightweight structural bricks have been investigated. XRD, XRF and TGA–DTA analysis of the waste and clay were performed. Samples containing up to 20 mass% spent earth from biodiesel filtration and up to 15 mass% glycerine have been fired at 1050 °C to produce pores and contribute to auto-thermal combustion due to its high heating power, which involves lower fuel consumption during firing step. Loss on ignition, linear shrinkage, bulk density, apparent porosity, water absorption, water suction, compressive strength, microstructural properties and thermal conductivity values of the fired samples were investigated. The results obtained showed that the use of waste decreased bulk density and increased apparent porosity of sintered samples. Values on mechanical properties decreased, due to the increase in water absorption and water suction, but were higher than those required by the standards. Thermal conductivity of the mixture brick decreased by 20% when spent earth from biodiesel filtration was incorporated, and up to a 40% when glycerine was added. Therefore, biodiesel waste is suitable as secondary raw materials in ceramic brick production.

13 ALTERNATIVE ENERGY SUPPLIES

Biofuels and bioconversion energy

13/01042 A critical review on additives to reduce ash related operation problems in biomass combustion applications

Wang, L. *et al. Energy Procedia*, 2012, 20, 20–29.

Biomass combustion has a huge potential to produce power and heat in a sustainable way. However, some biomass fuels have high potassium contents, which react with other ash forming elements (i.e. Cl, Si, P and S) and lead to different ash related operational problems. Utilization of additives to abate these problems have been studied and tested for several decades. This work reviews current knowledge and studies about properties and effects of additives reported in the literature. Various additives can mitigate ash-related issues by the following possible mechanisms: (1) capturing problematic ash species via chemical adsorption and reactions, (2) physical adsorption and elutriating troublesome ash species from combustion facilities, (3) increasing the biomass ash melting temperature by enhancing inert elements/compounds in ash residues, and (4) restraining biomass ash sintering by diluting and powdering effects from the additives. Additives are grouped according to the contained reactive compounds, including Al-silicates based additives, sulfur-based additives, calcium-based additives, and phosphorous-based additives. Additives with strong chemical adsorption and reaction capacities can minimize K-related ash sintering, deposition and slagging during biomass combustion processes. The effective chemical reaction mechanisms are closely related to K–Al–Si, K–Ca–Si and K–Ca–P systems. The capacities of additives to reduce ash-related problems are heavily influenced by mass/molar ratios between the reactive components in the additives and the problematic elements in the biomass ash, as well as the reaction atmosphere and combustion technology. More detailed studies on high temperature reactions between additives and ashes from biomass combustion are needed.

13/01043 A framework for model-based optimization of bioprocesses under uncertainty: lignocellulosic ethanol production case

Morales-Rodriguez, R. *et al. Computers & Chemical Engineering*, 2012, 42, 115–129.

This study presents the development and application of a systematic model-based framework for bioprocess optimization. The framework relies on the identification of sources of uncertainties via global sensitivity analysis, followed by the quantification of their impact on performance evaluation metrics via uncertainty analysis. Finally, stochastic programming is applied to drive the process development efforts forward subject to these uncertainties. The framework is evaluated on four different process configurations for cellulosic ethanol production including simultaneous saccharification and co-fermentation and separate hydrolysis and co-fermentation (SSCF and SHCF, respectively) technologies in different operation modes (continuous and continuous with recycle). The results showed that parameters related to pretreatment (e.g. activation energy of the reaction for glucose production, order of the reaction, etc.), hydrolysis (inhibition constant for xylose on conversion of cellulose and cellobiose, etc.) and co-fermentation (ethanol yield on xylose, inhibition constant on microbial growth, etc.), are the most significant sources of uncertainties affecting the unit production cost of ethanol with a standard deviation of up to US$0.13/gal-ethanol. Further stochastic optimization demonstrated the options for further reduction of the production costs with different processing configurations, reaching a reduction of up to 28% in the production cost in the SHCF configuration compared to the base case operation. Further, the framework evaluated here for uncertainties in the technical domain, can also be used to evaluate the impact of market uncertainties (feedstock prices, selling price of ethanol, etc.) and political uncertainties (such as subsidies) on the economic feasibility of lignocellulosic ethanol production.

13/01044 Application of a novel charge preparation approach to testing the autoignition characteristics of JP-8 and camelina hydroprocessed renewable jet fuel in a rapid compression machine

Allen, C. *et al. Combustion and Flame*, 2012, 159, (9), 2780–2788.

A variety of new, alternative jet fuels are being considered as replacements for conventional petroleum-derived jet fuels, and the autoignition chemistry of these fuels are of prime interest. However, traditional batch-based premixture preparation approaches used in chemical kinetics studies are burdened by the low volatility of these fuels. In this work, a new charge preparation approach is described and characterized in which a fuel and air premixture is created directly in the test chamber of a rapid compression machine. The approach relies on a fuel injector to load a small quantity of fuel into the test chamber with high resolution. Preparation of the test charge directly in the device rather than in a mixing vessel reduces the mixture pressure, and hence the fuel partial pressure and mixture temperature requirements to avoid thermal decomposition of the fuel. Gas chromatography/mass spectrometry is used to confirm that an accurately known mass of JP-8 jet fuel is injected into the rapid compression machine, and that all components of the fuel are evaporated and homogeneously mixed within 2 min of the fuel injection, for temperatures from 105 to 145 °C. Ignition delays for JP-8 in air are measured at low temperatures (670–750 K) and low pressures (7 and 10 bar) and the measurements are compared with literature data. The autoignition characteristics of the bio-based camelina hydroprocessed renewable jet fuel are also measured and contrasted with those of JP-8. Under similar compressed conditions, the camelina hydroprocessed renewable jet fuel ignition properties are distinct from JP-8, which provides motivation for pursuing new test strategies to elicit the autoignition chemistry of alternative jet fuels and other non-volatile fuels.

13/01045 Assessing the production of first and second generation bioethanol from sugarcane through the integration of global optimization and process detailed modeling

Furlan, F. F. *et al. Computers & Chemical Engineering*, 2012, 43, 1–9.
There is a worldwide effort to make economically feasible the use of lignocellulosic biomass for production of biofuels. In sugarcane industry, cane juice (sucrose) is fermented for bioethanol production. Sugarcane bagasse is used as fuel in cogeneration systems, to produce steam and electric power to the plant, and the surplus of electric power may be delivered to the grid. The hydrolysis of bagasse to produce second generation ethanol poses a challenge: how much bagasse can be diverted, since the process must continue energetically self-sufficient. This work presents a computational tool developed within an equation-oriented process simulator that couples the simulation of first and second generation bioethanol production with a global optimization algorithm. The tool was robust, optimizing the steady state process in any economic scenario and for different process configurations. Four case studies are presented, and their implications on process internal demands and on the surplus electrical power are discussed.

13/01046 Baseline effects on carbon footprints of biofuels: the case of wood

Johnson, E. and Tschudi, D. *Environmental Impact Assessment Review*, 2012, 37, 12–17.
As biofuel usage has boomed over the last decade so has research and regulatory interest in its carbon accounting. This paper examines one aspect of that carbon accounting: the baseline, i.e. the reference case against which other conditions or changes can be compared. A literature search and analysis identified four baseline types: no baseline, reference point, marginal fossil fuel and biomass opportunity cost. The fourth one, biomass opportunity cost, is defined in more detail, because this is not done elsewhere in the literature. The four baselines are then applied to the carbon footprint of a wood-fired power plant. The footprint of the resulting wood-fired electricity varies dramatically, according to the type of baseline. Baseline type is also found to be the footprint's most significant sensitivity. Other significant sensitivities are: efficiency of the power plant; the growth (or re-growth) rate of the forest that supplies the wood; and the residue fraction of the wood. Length of the policy horizon is also an important factor in determining the footprint. The paper concludes that because of their significance and variability, baseline choices should be made very explicit in biofuel carbon footprints.

13/01047 Bio-hythane production from food waste by dark fermentation coupled with anaerobic digestion process: a long-term pilot scale experience

Cavinato, C. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11549–11555.
In this paper are presented the results of the investigation on optimal process operational conditions of thermophilic dark fermentation and anaerobic digestion of food waste, testing a long-term run, applying an organic loading rate of 16.3 kgTVS/m^{3}d in the first phase and 4.8 kgTVS/m^{3}d in the second phase. The hydraulic retention times (HRTs) were maintained at 3.3 and 12.6 days, respectively, for the first and second phase. Recirculation of anaerobic digested sludge, after a mild solid separation, was applied to the dark fermentation reactor in order to control the pH in the optimal hydrogen production range of 5–6. It was confirmed the possibility to obtain a stable hydrogen production, without using external chemicals for pH control, in a long-term test, with a specific hydrogen production of 66.7 litre per kg of total volatile solid (TVS) fed and a specific biogas production in the second phase of 0.72 m^3 per kg TVS fed; the produced biogas presented a typical composition with a stable presence of hydrogen and methane in the biogas mixture around 6 and 58%, respectively, carbon dioxide being the rest.

13/01048 Bioavailability assessment of hexachlorobenzene in soil as affected by wheat straw biochar

Song, Y. *et al. Journal of Hazardous Materials*, 2012, 217–218, 391–397.
Biochar incorporation with soil could increase sorption of organic contaminants, thereby reducing their bioavailability. In this study, the effects of wheat straw biochar on the sorption, dissipation and bioavailability of hexachlorobenzene (HCB), a typical persistent organic pollutant (POP), were investigated in laboratory experiments. The authors observed that HCB sorption by biochar was 42 times higher than that by soil and the sorption isotherm was linear for the concentration range studied. Biochar amendments reduced HCB dissipation, volatilization and earthworm (*Eisenia foetida*) uptake of HCB from soil. Hydroxypropyl-β-cyclodextrin extraction correlated better with the earthworm bioassay than butanol extraction of HCB in biochar-amended soil. The results of both chemical extraction and earthworm bioassay indicate that biochar amendment of soil resulted in a rapid reduction in the bioavailability of HCB, even for the 0.1% biochar application rate. This suggested that wheat straw biochar could potentially be used in immobilizing POPs in contaminated sites.

13/01049 Biodiesel production by soybean oil methanolysis over SrO/MgO catalysts: the relevance of the catalyst granulometry

Dias, A. P. S. *et al. Fuel Processing Technology*, 2012, 102, 146–155.
The methanolysis of soybean oil was studied over magnesia supported SrO heterogeneous catalysts. The samples (0.05–0.35 Sr/Mg atomic ratio) were prepared by contacting commercial MgO with aqueous solutions of strontium nitrate. Both Mg and Sr oxides were identified by XRD even for the lowest Sr content. The calcination temperature is a critical issue for the catalytic performances because carbonated and hydroxylated surface species are only removed for calcination temperatures higher than 575 °C. Carbonated species seems to be more soluble in methanol than oxide species thus increasing the rate of Sr leaching. In tested conditions (67 °C, methanol/oil=9 and $W_{Cat}/W_{Oil}=5\%$) prepared catalysts presented interesting initial methanolysis activities. Catalysts with atomic ratios Sr/Mg higher than 0.10, showed analogous catalytic behaviours giving FAME (biodiesel) contents higher than 94%. The catalysts deactivation can be ascribable to strontium loss detected by XRD and SEM–EDS. The residual strontium remains trapped in MgO pores and thus inaccessible to the reactants. This result emphasizes the relevance of the external surface area of the catalysts due to the size of the triglycerides molecules and of the oil micelles, which cannot diffuse into catalysts pores. No soap formation was observed in the tested conditions.

13/01050 Biodiesel production from microalgae: co-location with sugar mills

Lohrey, C. and Kochergin, V. *Bioresource Technology*, 2012, 108, 76–82.
Co-location of algae production facilities with cane sugar mills can be a technically advantageous path towards production of biodiesel. Algal biodiesel production was integrated with cane sugar production in the material and energy balance simulation program *Sugars*^{TM}. A model was developed that allowed comparison of production scenarios involving dewatering the algae to 20% ds (dry solids) or 30% ds prior to thermal drying. The net energy ratio, E_R (energy produced/energy consumed) of the proposed process was found to be 1.5. A sensitivity analysis showed that this number ranged from 0.9 to 1.7 when the range of values for oil content, CO_2 utilization, oil conversion, and harvest density reported in the literature were evaluated. By utilizing available waste-resources from a 10,000 ton/d cane sugar mill, a 530 ha algae farm can produce 5.8 million L of biodiesel/yr and reduce CO_2 emissions of the mill by 15% without the need for fossil fuels.

13/01051 Biogas production from grape pomace: thermodynamic model of the process and dynamic model of the power generation system

Cáceres, C. X. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10111–10117.
In year 2010, the Province of San Juan in Argentina produced around 81,947 tons of grape pomace, which is a winery waste byproduct. Wineries demand a great quantity of power during the 3 months that winemaking time lasts, which involve a high installed electric power. This power is used mainly for refrigerating the must during the fermentation. The control of temperature is crucial in winemaking as the low temperature preserves subtle fruit characters. An alternative for reducing the requirement of power from the utility electric grid is producing it locally, using the residuals generated by the own wineries. The technology for bioenergy conversion proposed to be implemented

in this research for electricity generation is the anaerobic digestion of grape pomace. The aim of this research is to develop the thermodynamic equilibrium analysis of grape pomace anaerobic digestion based on the equilibrium constants for predicting the potential production of biogas and its composition. In addition, a dynamic model of a biogas-fuelled microturbine system for distributed generation applications is derived.

13/01052 CFD simulation of transient stage of continuous countercurrent hydrolysis of canola oil

Wang, W. C. *et al. Computers & Chemical Engineering*, 2012, 43, 108–119.

Computational fluid dynamic (CFD) modelling of a continuous countercurrent hydrolysis process was performed using ANSYS-CFX. The liquid properties and flow behaviour such as density, specific heats, dynamic viscosity, thermal conductivity, and thermal expansivity as well as water solubility of the hydrolysis components triglyceride, diglyceride, monoglyceride, free fatty acid, and glycerol were calculated. Chemical kinetics for the hydrolysis reactions were simulated in this model by applying Arrhenius parameters. The simulation was based on actual experimental reaction conditions including temperature and water-to-oil ratio. The results not only have good agreement with experimental data but also show instantaneous distributions of concentrations of every component in hydrolysis reaction. This model provided visible insight into the continuous countercurrent hydrolysis process.

13/01053 Characterising biofuels and selecting the most appropriate burner for their combustion

San José Alonso, J. F. *et al. Fuel Processing Technology*, 2012, 103, 39–44.

This paper presents the results obtained in the combustion of samples of biofuels using a commercial burner. Analysis of biofuels has shown that in comparison to diesel, biofuels evidence: (i) a lower lower heat value, (ii) a high percentage of oxygen in their composition, (iii) a greater density, and (iv) much higher viscosity. All of this leads to the conclusion that biofuels cannot use the same burners as are used to burn diesel. The criterion used to select the burner based on the pulverization of the fuel and its stability depending on the density and viscosity of the fuel can be considered acceptable for oils but not for fats due to problems of flame stability and particle emissions. Combustion of vegetable oils is totally feasible and provides similar results to diesel combustion with regard to emission levels, combustion efficiency and reduction of greenhouse gases. The present work highlights the possibility of burning the biofuels that exist on the market using available technologies without the need to make large investments.

13/01054 Continuous production of biodiesel using whole-cell biocatalysts: sequential conversion of an aqueous oil emulsion into anhydrous product

Yoshida, A. *et al. Biochemical Engineering Journal*, 2012, 68, 7–11.

A continuous production of biodiesel from an aqueous plant oil emulsion was attempted using immobilized fungal whole cells. Six packed-bed reactors were connected in series and operated with stepwise methanol addition. In the first column, more than 3% water was necessary for methanolysis to proceed. Despite the low initial water content of 0.36%, the methyl ester content in the effluent from the second column increased similarly in a wide range of contents of water (0–20%) added, which shows the water-content-independent reaction in this column in contrast to the reaction in the first column. Further investigations using reaction mixture models suggested a contribution of the composition of the reaction mixture to the phenomenon. On the basis of these findings, the sequential methanolysis through six columns was attempted, where the upper layer of the effluent from each column was supplied into the next column without further addition of water. Consequently, an aqueous plant oil emulsion with 3% water was converted into the final product with 96.1% methyl ester and 0.15% water. Therefore, the system developed is useful for producing biodiesel enzymatically from water-containing feedstocks.

13/01055 Corrosion of ceramics for vinasse gasification in supercritical water

Richard, T. *et al. Journal of the European Ceramic Society*, 2012, 32, (10), 2219–2233.

Supercritical water gasification (SCWG) is a very efficient process to convert wet biomass into energetic gases. Unfortunately, SCWG reactor may strongly corrode due to the addition of temperature, pressure and the presence of corrosive species. In the present paper, the corrosion of various ceramic materials in subcritical and supercritical water gasification process was studied in a batch reactor. The authors compared the corrosion in distilled water and the corrosion in sugar beet slurry that will be gasified under supercritical conditions. The experimental temperatures were 350 and 550 °C and the pressure was 25 MPa. Technical ceramics (SiC, alumina, Y-stabilized zirconia, Si_3N_4, BN, aluminosilicate, cordierite-mullite) show poor capability to sustain corrosion whereas graphite and glassy carbon are the highest performance materials in the working conditions.

13/01056 Decarboxylation of microalgal oil without hydrogen into hydrocarbon for the production of transportation fuel

Na, J. G. *et al. Catalysis Today*, 2012, 185, (1), 313–317.

A catalytic decarboxylation process following pyrolysis was developed for the production of transportation fuels from microalgae. The pyrolysis of *Chlorella* sp. KR-1, which has a triglyceride content of 36.5%, was carried out at 600 °C to obtain feedstock oil for decarboxylation. The major compounds in the pyrolysis oil were free fatty acids with carbon numbers of 16 and 18. Decarboxylation of the pyrolysis oil was performed using a type of hydrotalcite (MG63) as a catalyst at temperatures of 350 °C and 400 °C. Due to the selective reaction by MG63, hydrocarbons with carbon numbers of 15 and 17 were the most abundant compounds in the liquid product. The product yield at a reaction temperature of 400 °C was 78.6% and the degree of oxygen removal was 78.0%. Inert or less active oxygenates for hydrotalcite, such as phenolic compounds and fatty acid alkyl ester, may prevent the complete removal of oxygen. The diesel fraction in the product obtained under the given reaction condition was 83.8%, whereas that of the pyrolysis oil was 35.5%.

13/01057 Direct production of biodiesel from rapeseed by reactive extraction/in situ transesterification

Zakaria, R. and Harvey, A. P. *Fuel Processing Technology*, 2012, 102, 53–60.

Biodiesel is a fuel derived from renewable resources such as edible and inedible oil-bearing seed, algae, and waste cooking oil. The conventional biodiesel process involves oil extraction, refining and transesterification. Alternatively, transesterification can actually be performed directly from the oil-bearing materials without prior extraction. This route which is often termed ‘reactive extraction’ or ‘*in situ* transesterification’ has the advantages of simplifying the biodiesel production process as well as potentially reducing production cost. In this study, the reactive extraction of rapeseed with methanol has been characterized. The effects of process parameters on the yield, conversion and reaction rate differ substantially from conventional transesterification due to the dependence on both extraction and reaction. The rate of ester formation is mainly affected by the catalyst concentration, temperature and particle size while the equilibrium yield largely depends on the solvent to oil molar ratio. A high yield of ester (>85%) can only be achieved at high solvent to oil molar ratios (>475:1). Parametric studies and light microscope images of reactively extracted seed suggested that reactive extraction occurs by transesterification of the oil inside the seed, followed by diffusion of the products into the bulk solvent.

13/01058 Efficacy of gossypol as an antioxidant additive in biodiesel

Moser, B. R. *Renewable Energy*, 2012, 40, (1), 65–70.

The efficacy of gossypol as an antioxidant additive in fatty acid methyl esters (FAMEs) prepared from soybean oil (SME), waste cooking oil (WCME) and technical grade methyl oleate (MO) was investigated. Gossypol is a naturally occurring polyphenolic aldehyde with antioxidant properties isolated from cottonseed that is toxic to humans and animals. At treatment levels of 250 and 500 ppm, gossypol exhibited statistically significant improvements in the induction periods (IPs; EN 14112) of SME, WCME and MO. Efficacy was most pronounced in SME, which was due to its higher concentration of endogenous tocopherols (757 ppm) versus WCME (60 ppm) and MO (0 ppm). A comparison of antioxidant efficacy was made with butylated hydroxytoluene (BHT) and γ-tocopherol. For FAMEs with low concentrations of endogenous tocopherols (WCME and MO), γ-tocopherol exhibited the greatest efficacy, although treatments employing BHT and gossypol also yielded statistically significant improvements to oxidative stability. In summary, gossypol was effective as an exogenous antioxidant for FAMEs investigated herein. In particular, FAMEs containing a comparatively high percentage of endogenous tocopherols were especially suited to gossypol as an antioxidant additive.

13/01059 Environmental treatment of slaughterhouse wastes in a continuously stirred anaerobic reactor: effect of flow rate variation on biogas production

Marcos, A. *et al. Fuel Processing Technology*, 2012, 103, 178–182.

The present study shows the treatment of slaughterhouse wastes of Badajoz municipal in Spain by an anaerobic codigestion process. The experimental device used was a completely mixed type (6-litre capacity) continuous biodigester with recirculation of the methane produced in the anaerobic digestion. Under mesophilic conditions (37 °C), the biological anaerobic degradation, biogas production, and inhibition processes were analysed for six flow rates; 200, 275, 350, 400, 537 and 672 ml/day. It was found that the environmental optimum flow rate is 350 ml/day for energy production.

13/01060 Fuel-nitrogen conversion in the combustion of small amines using dimethylamine and ethylamine as biomass-related model fuels

Lucassen, A. *et al. Combustion and Flame*, 2012, 159, (7), 2254–2279.

Laminar premixed flames of the two smallest isomeric amines, dimethylamine and ethylamine, were investigated under one-dimensional low-pressure (40 mbar) conditions with the aim to elucidate pathways that may contribute to fuel–nitrogen conversion in the combustion of biomass. For this, identical flames of both fuels diluted with 25% Ar were studied for three different stoichiometries ($\Phi = 0.8$, 1.0, and 1.3) using *in situ* molecular-beam mass spectrometry (MBMS). Quantitative mole fractions of reactants, products and numerous stable and reactive intermediates were determined by electron ionization (EI) MBMS with high mass resolution to separate overlapping features from species with different heavy elements by exact mass. Species assignment was assisted by using single-photon vacuum-ultraviolet (VUV) photoionization (PI) MBMS. The results indicate formation of a number of nitrogenated intermediates, including toxic species such as HCN, in appreciable concentrations. Such intermediate species mole fractions may depend not only on stoichiometry, but also on fuel structure. The authors attempted to analyse the major pathways in the two flames with a detailed combustion model developed for this purpose. For this, thermochemical values for a number of intermediates had to be determined from quantum chemistry calculations. Also, specific sets of reactions were incorporated for the two fuels. While many trends seen in the experiments can be successfully reproduced by the simulations, additional efforts may be needed to reliably describe the fuel-nitrogen chemistry in the combustion of biomass-related model fuels with amine functions.

13/01061 Gasification of biomass in a fixed bed downdraft gasifier – a realistic model including tar

Barman, N. S. *et al. Bioresource Technology*, 2012, 107, 505–511.

This study presents a model for fixed bed downdraft biomass gasifiers considering tar also as one of the gasification products. A representative tar composition along with its mole fractions, as available in the literature was used as an input parameter within the model. The study used an equilibrium approach for the applicable gasification reactions and also considered possible deviations from equilibrium to further upgrade the equilibrium model to validate a range of reported experimental results. Heat balance was applied to predict the gasification temperature and the predicted values were compared with reported results in literature. A comparative study was made with some reference models available in the literature and also with experimental results reported in the literature. The results obtained by the model showed fairly good agreement with results from the reference model as well as with the experimental investigations. This study has successfully shown that, if the tar mass is accounted for in the mass balance, the rest of the gasification product (permanent gas species, including moisture vapour) may be predicted with considerable degree of accuracy by simple equilibrium model, considered with deviation from the equilibrium for the methane reaction.

13/01062 Hydrolysis kinetics characteristic of recycled fiber in subcritical water

Wang, Y. *et al. Bioresource Technology*, 2012, 105, 152–159.

Recycled fibre hydrolysis was conducted to evaluate the feasibility of reducing sugar accumulation for biofuel products during hydrolysis in subcritical water. The hydrolysis conversion of recycled fibre was reaching to approximate 90% within 3 min at 280–320 °C, while the glucose decomposed simultaneously within 0.5 min. The FTIR wave variation and the crystalline index of hydrolysis residue indicated that the intermolecular, intramolecular hydrogen bond and the crystalline was a constraint for recycled fibre hydrolysis. The kinetics analysis demonstrated the cylindrical shape model is proper at low temperature for recycled fibre hydrolysis, while sphere shape model is suitable at high temperature. The apparent activation energies of recycled fibre on both kinetics models were 58.19 and 53.18 kJ mol^{-1}, which were lower than that the glucose with 79.59 kJ mol^{-1}. Therefore, the conclusion is drawn that the high yield of glucose during recycled fibre hydrolysis is achievable by reducing the cellulose crystalline through proper indispensable pretreatments.

13/01063 Hydrothermal carbonization as an effective way of densifying the energy content of biomass

Román, S. *et al. Fuel Processing Technology*, 2012, 103, 78–83.

Hydrothermal carbonization processes were studied under different conditions using two different biomass materials: walnut shell and sunflower stem. Coalification under mild conditions was promoted with the aim of increasing the calorific value of the solid hydrochar. Hydrocarbonization processes brought up an increase on the heating value of the materials up to 28.9 and 29.3 MJ kg^{-1}, for sunflower stem and walnut shell, respectively, which corresponds to an increase of 1.75 and 1.50 fold when compared with the natural biomass. Also, regarding the variables studied it was found that temperature and water/biomass ratio were more influent on the hydrocarbonization process than residence time. The hydrochars show negligible N_2 adsorption at 77 K and interesting surface morphology, characterized by the formation of microspheres which grow as temperature increases. Moreover, hydrochars are acid in nature and present several oxygen functionalities, as observed from FT-IR and pzc analysis.

13/01064 Improved operating policy utilizing aerobic operation for fermentation process to produce bio-ethanol

Chang, D. M. *et al. Biochemical Engineering Journal*, 2012, 68, 178–189.

To enhance the productivity of the alcohol fermentation process, combined aerobic and anaerobic fed-batch operation could improve the growth of microbes and also achieve better alcohol production because of well-utilizing the characteristics of the microbial metabolism. Using a realistic model fitted from experimental data, result shows that the highest productivity can be achieved using a proposed fed-batch operation with high glucose concentration. The proposed operating policy combines an initial aerobic operation to increase the biomass formation in the early phase of the fed-batch operation and then followed by the anaerobic operation to accelerate the alcohol production in the later phase. The glucose feeding policy for this optimal fed-batch operation should try to maintain a lower optimal glucose concentration in the fermenter during initial aerobic phase and then to maintain another higher optimal glucose concentration during the next anaerobic phase. Toward the ending of the fed-batch, the glucose concentration in the fermenter should be increased further in order to speed up the productivity of ethanol after the feeding stopped.

13/01065 Innovative biogas multi-stage biogas plant and novel analytical system: first project experiences

Moedinger, F. *et al. Energy Procedia*, 2012, 18, 672–680.

A research network formed by Renergia, Metalinox (project leader), University of Trento and University of Trier has been established in order to build and operate a multi-stage type research fermenter system to explore the potential of a multi-stage fermentation system. The expected results of this project are clearly targeted at improving the specific gas yield, introducing, for the biogas sector, new analytical methods and novel methods of disposal of the solid fermentation wastes. The project as presented here will hence be a substantial contribution to new knowledge and know-how. The first operational results of the R&D plant are, at the time of writing of this paper, not yet available for publication and the collected data will be source for later publication. Building R&D scaled plants in the anaerobic digestion sector as proof of concept is a rather uncommon approach for the sector: Almost always laboratory results are transferred directly to full size plant level. Many times this approach results in failure as the operational conditions under which data are obtained are not comparable. Many times novel substrate, as an addition or substitution of the existing substrate, are tested experiencing a drop in the production of biogas and hence generation of energy. With the R&D plant it will also be easier to test, verify and improve the novel analytical methods. In a full-size commercial plant it would be unthinkable to establish certain operational conditions, intentionally presumably wrong density and temperature of the substrate for example, that are required and necessary to fine tune the analytical method and verify the operational parameters that result from the analysis. Scaling up the experiences made with the R&D plant will help in avoiding mistakes both in design and process control. The R&D plant will also be a valuable asset once a full scale plant has been built as a test bed for certain substrates that might be deemed to be used in the full-size plant in order to optimize and determine process parameters before the new or additional substrate is fed to the commercial size plant. Even from a purely financial point of view such a novel approach will certainly be, in a period of time where public incentives are decreasing, important and highly desirable.

13/01066 Materials flow modeling of nutrient recycling in biodiesel production from microalgae

Rösch, C. *et al. Bioresource Technology*, 2012, 107, 191–199.

Biodiesel production based on microalgae as feedstock is associated with a high demand of nutrients, respectively nitrogen and phosphorus. The production of 1 litre of biodiesel requires between 0.23 and 1.55 kg nitrogen and 29–145 g of phosphorus depending of the cultivation conditions for microalgae. The supply of nutrients can be expected to severely limit the extent to which the production of biofuels from microalgae can be sustainably expanded. The nutrient demand can be reduced if the nutrients in the residual algae biomass after oil extraction are reused for algae cultivation. This modelling work illustrates that for the investigated process chains and scenarios the nutrient recycling rates are in the range from 30% to 90% for nitrogen and from 48% to 93% for phosphorus. The highest recycling values can be achieved by hydrothermal gasification of the oil-free residues.

13/01067 Mathematical modeling of process liquid flow and acetoclastic methanogenesis under mesophilic conditions in a two-phase biogas reactor

Muha, I. *et al. Bioresource Technology*, 2012, 106, 1–9.

Acetoclastic methanogenesis in the second stage of a two-phase biogas reactor is investigated. A mathematical model coupling chemical reactions with transport of process liquid and with the variation of population of the microorganisms living on the plastic tower packing of the reactor is proposed. The evolution of the liquid is described by an advection–diffusion–reaction equation, while a monod-type kinetic is used for the reactions. Moreover, a new inhibition factor MO_{max} is introduced, which hinders the growth of microorganisms when the plastic tower packing is overpopulated. After estimating the reaction parameters, the acetate outflow measured experimentally is in good agreement with that predicted by simulations. For coupling liquid transport with reaction processes, a spatial discretization of the reactor is performed. This yields essential information about the distribution of acetate and the production of methane in the reactor. This information allows for defining a measure of the effectiveness of the reactor.

13/01068 Mechanistic and kinetic investigations in ultrasound assisted acid catalyzed biodiesel synthesis

Parkar, P. A. *et al. Chemical Engineering Journal*, 2012, 187, 248–260.

This paper attempts to discern physical mechanism and kinetic aspects of ultrasound irradiation on transesterification of soybean oil with methanol using sulfuric acid as catalyst with approach of coupling experimental results with simulations of cavitation bubble dynamics. Kinetic constants as well as activation energies of transesterification reaction were determined at different alcohol to oil molar ratios and reaction temperatures. The results of this study reveal interesting features of the relationship between mechanics of ultrasound/cavitation, and the intrinsic behaviour (represented by specific rate constant) of the transesterification reaction. The beneficial effect of ultrasound irradiation on transesterification is of physical nature. Several anomalies of ultrasound-assisted acid catalysed transesterification (as compared to conventional system) are: occurrence of reaction at low temperature of 15 °C (albeit with low conversions of 13.45% and 10.2% for alcohol to oil molar ratios of 6:1 and 12:1, respectively); despite higher activation energy, higher rate constant at low alcohol to oil molar ratio of 6:1; and minima shown by reaction rate constant with temperature. The major physical effect of sonication is fine emulsification that generates enormous interfacial area for reaction that overwhelms the effect of specific rate constant. As revealed by simulations, physical effects of cavitation (namely, micro-convection and shock waves) are more pronounced at low temperature, which is primary cause leading to these anomalies.

13/01069 Microstructure of carbon molecular sieve membranes and their application to separation of aqueous bioethanol

Liao, K. S. *et al. Carbon*, 2012, 50, (11), 4220–4227.

Pyrolytic carbons were fabricated from a Kapton precursor. The microstructure of the carbon molecular sieve membranes (CMSMs) was examined by means of sorption tests using pure liquid sorbates of different molar volumes and with the application of positron annihilation lifetime spectroscopy (PALS). The pore sizes of the CMSMs were calculated by PALS and the recently proposed equation relating positron lifetime with free volume radius. The mean pore radius in the CMSMs was demonstrated to be smaller than 3 Å. Their ability to separate water from bioethanol was determined. Results of aqueous bioethanol sorption showed evident molecular sieving behaviour of the CMSMs despite their hydrophobic surface. This behaviour became significant at a high pyrolysis end temperature of 700 °C, at which the carbon content was high. The c700 membrane delivered a high permeation flux of $1199\,\mathrm{g/m^2\,h}$ and a high separation factor of 683. This performance suggests that CMSMs have more potential to separate water from bioethanol through pervaporation or vapour permeation than organic membranes.

13/01070 New method for assessing the performance of agricultural biogas plants

Djatkov, D. *et al. Renewable Energy*, 2012, 40, (1), 104–112.

Around 5000 agricultural biogas plants were operating in Germany by the end of 2009. There is a recognized need for their assessment, comparison and performance improvement. Prerequisites for their reliable assessment include: (1) detailed and reliable performance data, (2) defined criteria for the assessment, and (3) a comprehensive method. The limitations of existing assessment methods have been reviewed. The new method developed for assessing the overall performance of biogas plants is focused on four assessment aspects: biogas production, biogas utilization, environmental impact and socio-economic efficiency. Each assessment aspect was determined by two performance criteria. The method is based on fuzzy set theory and fuzzy mathematics, which enables use of imprecise and uncertain data. Incorporation of enough expertise from the field of biogas technology was enabled in this method as well. Pre-assessment of future biogas plants in their planning phase is possible, contributing to their effective development. The reliability of the method was tested using data from 10 monitored biogas plants. The assessment of the 10 biogas plants showed that biogas utilization is the aspect with the largest potential for performance improvement, by increasing the external heat utilization. The method developed is adjustable to accommodate new developments related to biogas technology and biogas plants in any geographical region. Future research should be focused on definition and inclusion of more assessment criteria and on developing the methods that are capable to handle compensation between individual criteria.

13/01071 Novel mesoporous silica supported ZnO adsorbents for the desulphurization of biogas at low temperatures

Hussain, M. *et al. Chemical Engineering Journal*, 2012, 188, 222–232.

Biogas, a valuable renewable energy carrier, can be used as a fuel or as a raw material for the production of synthesis gas and hydrogen. However, the significant quantities of undesirable contaminants, especially hydrogen sulfide (H_2S), constitute process problems and also generate harmful environmental emissions. The key objective of this work was to develop an adsorbent system for the H_2S desulfurization of biogas at ambient temperature, which would be capable of reducing H_2S to less than 1 ppmv in order to achieve high removal efficiency (>99%). The potential of MCM-41, KIT-6, SBA-15-Spherical type (SBA-15-S) and SBA-15-Fibre type (SBA-15-F) supported ZnO adsorbents has been explored at ambient temperature for H_2S desulfurization in order to develop a more effective adsorbent for this important application. ZnO loadings of 10, 15 and 20 wt% were impregnated by the incipient wetness method to achieve mesoporous silica supported ZnO adsorbents. The adsorbents were characterized by N_2 adsorption/desorption, using the BET method and the field emission scanning electron microscope (FESEM) technique, to investigate their various characteristics. 15 wt% ZnO supported on MCM-41/, KIT-6/, SBA-15-S/or SBA-5-F showed a higher adsorption capacity than 10 or 20 wt% ZnO loadings, this might be due to the smaller size of the ZnO particles in dispersed form with improved loading. However, the adsorption capacity decreased, at a higher loading of 20 wt% of ZnO, because of the increased particle size which is due to agglomerated dispersed form. The SBA-15-F and SBA-15-S supported ZnO showed better desulfurization performances than MCM-41, KIT-6 or the widely adopted commercial activated carbon material ROZ3 and commercial or synthesized titania supported ZnO adsorbents, due to their retained superior physical properties as well as to the size and dispersion of ZnO on the surface of these materials.

13/01072 Oil productivity of the tropical marine diatom *Thalassiosira* sp.

Nurachman, Z. *et al. Bioresource Technology*, 2012, 108, 240–244.

To understand the potential of cultivating tropical marine diatom *Thalassiosira* sp. to produce biofuel, biodiesel product properties and growth characteristics of *Thalassiosira* sp. in three different media were investigated. After medium evaluation, significant *Thalassiosira* sp. cell growth was observed in both Walne and enriched seawater media, but not in plain seawater medium. The microalgae grew well in alkaline condition (pH range of 8.0–8.8). The average biomass density cultured in Walne and enriched seawater media on the sixth day was 4.36 and $2.50\,\mathrm{g\,L^{-1}}$, respectively. Based on ESI-IT-MS spectra, the TAGs of algal oil were identified as POP, POO and SOO, and the FAMEs as oleic acid methyl ester. The oil productivity of *Thalassiosira* sp. cultured in Walne and enriched seawater media were 150 and $290\,\mu\mathrm{L\,L^{-1}\,d^{-1}}$, respectively. The density and kinematic viscosity of *Thalassiosira* sp. biodiesel were $0.857\,\mathrm{g\,mL^{-1}}$ and $1.151\,\mathrm{mm^2\,s^{-1}}$.

13/01073 Purification of bioethanol using extractive batch distillation: simulation and experimental studies

Pacheco-Basulto, J. Á. *et al. Chemical Engineering and Processing: Process Intensification*, 2012, 61, 30–35.

Among biofuels, bioethanol has increased in importance in many countries because it can be used directly or mixed with gasoline in combustion engines. The production of bioethanol in a fermentative process usually gives a dilute solution from which the bioethanol must be obtained in high concentration in order to be used as biofuel. The separation of an azeotropic mixture of ethanol and water using batch and semi-batch distillation was studied considering ethylene glycol and ionic liquids as entrainers. The simulation and experimental results indicate that the separation is favoured using ethylene glycol in comparison to the use of ionic liquid; however, the ionic liquid is considered a green solvent and the use of ethylene glycol could be forbidden in the near future.

13/01074 Sliding mode observer for biomass estimation in a biohydrogen production process

Nuñez, S. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10089–10094.

This work deals with the problem of estimation of biomass concentration and specific growth rate in a biohydrogen production process. A photo-fermentation process with the photosynthetic bacteria *Rhodobacter capsulatus* is considered. The reaction dynamics is represented with a Monod law while the hydrogen production rate is modelled with a Luedeking–Piret expression. A sliding mode observer is proposed and designed, which gives an estimate of both biomass concentration and specific growth rate from measurements of the produced hydrogen volume. The proposed observer is completely robust against the growth kinetic model, and it presents a first-order reduced dynamics. Numerical simulation results are presented for a batch biohydrogen production process.

13/01075 Study of products yield of bagasse and sawdust via slow pyrolysis and iron-catalyze

Lin, T. Y. and Kuo, C. P. *Journal of Analytical and Applied Pyrolysis*, 2012, 96, 203–209.

In this paper, the slow pyrolysis behaviour of the bagasse and sawdust was studied at the different heating rates, the different iron-containing blend pyrolysis and the treatment temperature, the further understood for the pyrolysis of agricultural residues. The distribution of the products yield of the slow pyrolysis process, it is typically performed at temperature between 200 and 600 °C, the pyrolysis temperature increased, the bio-liquids and gas yields tended to increase, which at 400 °C was able to achieve maximum bio-liquids yields, the biochar yields tended to downward. For different heating rate, in the heating rate ranges for 80–100 W, the bio-liquids products yield curve increased from 44.5 to 46.5 wt% for bagasse; the sawdust products yield increased from 41 to 42.75 wt%. Iron-catalysts blend pyrolysis (0, 10, 25, 40 and 50 wt%), the bagasse bio-liquid yields respectively 56.25 wt% in the presence 50% iron-catalysts blend pyrolysis; the sawdust bio-liquid yields respectively 52.5 wt% in the presence 40% iron-catalysts blend. The pyrolysis process were calculated according to the kinetic mechanism were examined, the pyrolysis activation energy was between 6.55 and 7.49 kcal/mol for bagasse. Sawdust the pyrolysis activation energy was between 11.52 and 11.76 kcal/mol. Therefore, in this study a pyrolysis model of bagasse and sawdust thermal treatment may provide both agricultural and forestry transformation importance of resources.

13/01076 Transesterification of castor oil under ultrasonic irradiation conditions. Preliminary results

Encinar, J. M. *et al. Fuel Processing Technology*, 2012, 103, 9–15.

In this work, the preliminary results obtained in the transesterification of castor oil with methanol in the presence of ultrasonic irradiations, are presented. The fundamental objective was to study the acceleration that the ultrasound causes in the reaction rate. The effect of different operating variables, such as frequency and supplied power dissipation, catalyst (KOH) concentration and methanol oil molar ratio were also investigated. The evolution of the process was followed by gas chromatography, determining the concentration of the methyl esters at different reaction times. The biodiesel was characterized by its density, viscosity, saponification value, iodine value, acidity index, water content, flash point, combustion point, cetane index and cold filter plugging point (CFPP), according to ISO norms. Between these properties, viscosity, the number of cetane and the CFPP do not attain the values established by the standard EN 14214. These circumstances would force to use the castor biodiesel oil mixed with diesel fuel oil, or to add additives in order that the previous properties reach the specified values. High methyl ester yield and fast reaction rate could be obtained, for castor oil transesterification, under ultrasonic conditions, even if the reaction temperature was relatively low. In general, the variables of operation tested exercise a positive effect on the reaction rate, but the obtained final yield (equilibrium) is very similar in all cases.

13/01077 Wavelength specificity of growth, photosynthesis, and hydrocarbon production in the oil-producing green alga *Botryococcus braunii*

Baba, M. *et al. Bioresource Technology*, 2012, 109, 266–270.

The effect of monochromatic light on growth, photosynthesis, and hydrocarbon production was tested in *Botryococcus braunii* Bot-144 (race B), which produces triterpenoid hydrocarbons. The growth was higher in order of red, blue and green light. The colour of red light-grown cells became more orange–yellow and their shape dominantly changed to grape-like with long branches. Photosynthetic carbon fixation activity was higher in order of blue, red, and green light-grown cells, but photosystem activities showed no difference. In the pulse-chase experiments with $^{14}CO_2$, no major difference was observed in the production of lipids, hydrocarbons, polysaccharides, or proteins among the three kinds of cells, although hydrocarbon production was slightly lower in green light-grown cells. These results indicate that blue and red light were more effective for growth, photosynthetic CO_2 fixation, and hydrocarbon production than green light, and that red light is the most efficient light source when calculated based on photoenergy supplied.

13/01078 Yield and physicochemical properties of mechanically extracted crude *Jatropha curcas* L oil

Tambunan, A. H. *et al. Biomass and Bioenergy*, 2012, 43, 12–17.

Knowledge on physical properties and their dependence on moisture content of *Jatropha curcas* L. seeds are essential to improve the design of equipment for harvesting, processing and storage of the seeds. The objective of this experiment is to find the effect of mechanical extraction method to the physicochemical properties of the extracted oil. The result is expected to be valuable as basic data for designing the equipment and process related to the extraction of oil from the seed of jatropha. The oil extraction was performed using a specially designed laboratory scale mechanical extractor, and the yield was calibrated with soxhlet apparatus using hexane as the solvent to obtain its extraction efficiency. The experiment was conducted in factorial arrangement, with four types of sample (seeds, kernel, crushed seeds, and crushed kernel), four extraction temperature (ambient, 50, 60 and 80 °C), and three preheating time (600, 1200 and 2400 s), and analysed with Duncan multiple range test. The results show that crushing the kernel of jatropha before extracting the oil mechanically will give higher oil yield and higher extraction efficiency. Higher temperature and longer preheating time also increase the oil yield. However, the maximum applicable temperature for mechanical extraction is 60 °C, since the viscosity and free fatty acid content of the extracted oil will increase if the extraction temperature increased above the temperature.

Geothermal energy

13/01079 A novel integrated system of ground heat exchanger and indirect evaporative cooler

Khalajzadeh, V. *et al. Energy and Buildings*, 2012, 49, 604–610.

Thermal analysis of a novel integrated system of ground heat exchanger and indirect evaporative cooler is performed in the summer conditions of Tehran, the capital city of Iran. A ground-coupled circuit pre-cools the entering air of an indirect evaporative cooler. This circuit includes four vertical ground heat exchangers which are arrayed in a series configuration. In order to have an accurate prediction of the optimum performance of the ground-coupled circuit, a three-dimensional computational fluid dynamics simulation is run. The simulation results reveal that the combination of the ground-coupled circuit and the indirect evaporative cooler can easily provide comfort conditions. Based on the results, the cooling effectiveness of this hybrid system is more than unity and this novel hybrid system significantly decreases the air temperature below the ambient wet-bulb temperature. As a result, the proposed system can be used as a clean and efficient air conditioner.

13/01080 Cascade utilization of low temperature geothermal water in oilfield combined power generation, gathering heat tracing and oil recovery

Li, T. *et al. Applied Thermal Engineering*, 2012, 40, 27–35.

Oil wells at the high water-cut stage are used as geothermal wells and geothermal power plants in oilfield have their own advantages. A new compound system combining the organic Rankine cycle (ORC) plant with the gathering heat tracing (GHT) station and the oil recovery system is presented. First, the exergy destruction of the system is calculated and the reason for the low efficiency of the ORC with R123 is pinpointed through exergetic analysis. The plant is optimized numerically and working fluids investigated are R601a, R601, R123, R141b, R245fa and R600. A new objective function is defined, reflecting both technical and economic performances. The feasibility of replacing oil boilers with geothermal water is then analysed. Finally, the overall economic performance is calculated. Results show that the exergy destruction of the ORC with R123 is the highest. The optimized plant with R601a increases the net power output by about 40%. About 8163 tons of oil is saved and about 34,600 tons of oil is recovered per year. The payoff period is only about 3.2 years whereas it will be sharply shortened if the earnings of oil are also considered. The new system is rational in technology and profitable in economy, which can be used as a way to increase economic benefits for oilfields at the high water-cut stage.

13/01081 Geochemical and geo-electrical study of mud pools at the Mutnovsky volcano (South Kamchatka, Russia): behavior of elements, structures of feeding channels and a model of origin

Bessonova, E. P. *et al. Applied Geochemistry*, 2012, 27, (9), 1829–1843.

This study presents data on the geochemical composition of boiling mud pools at the Mutnovsky volcano. The physicochemical characteristics of the pools and the concentrations of major, minor and trace elements in pool solutions vary widely. A comparison of the geochemical compositions of host rocks and solutions indicates that leaching from rocks is not the only source of chemicals in thermal solutions. Geophysical studies reveal the inner structure of thermal fields, which reflect the shapes of the underground reservoirs and feed channels. Using geophysical methods (electrical resistivity tomography and frequency domain investigations), it was shown that the vertical structure and complex geochemical zonation of the feed channels leads to a high contrast in the compositions of the mud solutions. These findings answer questions about the origin and composition of surface manifestations. To elucidate the mechanisms of solution formation, an attempt was made to describe the magmatic fluid evolution and the resulting mixing of waters by physical and mathematical models. The model illustrates fluid migration from a magma chamber to the surface. It is shown that the formation of brines corresponding to the mud pool composition is possible during secondary boiling.

13/01082 Geothermal energy production utilizing abandoned oil and gas wells

Bu, X. *et al. Renewable Energy*, 2012, 41, 80–85.

The objective of this study is to demonstrate the feasibility of acquiring geothermal energy from existing abandoned oil and gas wells. The equations describing the heat exchange between fluid and rocks are developed, and parametric studies are conducted in order to specify the optimum values of the main parameters. Computational results indicate that the geothermal energy produced from abandoned wells depends largely on the flow rate of fluid and the geothermal gradient. The temperature of extracted liquid is 129.88 °C, and it drops to 127.92 °C after 10 years of operation. It is observed that both hot water and electricity can be acquired from the abandoned wells. Results also indicate that the distance of two wells should not be less than 40 m in order to avoid interaction between them. Furthermore, the financial reward of electricity is US$36,833.26/year for a retrofitted well.

13/01083 Hydrogeochemistry of high-temperature geothermal systems in China: a review

Guo, Q. *Applied Geochemistry*, 2012, 27, (10), 1887–1898.

As an important part of the Mediterranean-Himalayas geothermal belt, southern Tibet and western Yunnan are the regions of China where high-temperature hydrothermal systems are intensively distributed, of which Rehai, Yangbajing and Yangyi have been investigated systematically during the past several decades. It has been confirmed by studies on Cl^- and stable isotope geochemistry that magma degassing makes an important contribution to the geothermal fluids from Rehai, Yangbajing and Yangyi, though meteoric water is still the major source of recharge for these hydrothermal systems. However, the mechanisms of magma heat sources appear to be quite different in the three systems, as recorded by the $^3He/^4He$ ratios of escaping geothermal gases. A mantle-derived magma intrusion to shallow crust is present below Rehai, although the intruding magma has been heavily hybridized by crustal material. By contrast, the heat sources below Yangbajing and Yangyi are inferred to be remelted continental crust. Besides original sources, the geochemistry of characteristic constituents in the geothermal fluids have also been affected by temperature-dependent fluid–rock interactions, boiling and redox condition changes occurring in the upper part of hydrothermal systems, and mixing with cold near-surface waters. The geothermal fluids from Rehai, Yangbajing and Yangyi contain very high concentrations of some toxic elements. Since local drinking water sources may be mixed with geothermal water, and irrigation with water containing geothermally derived harmful elements, possibly leading to accumulation in crops consumed by human beings, the natural geothermal spring discharge or anthropogenic geothermal wastewater drainage of these fields poses a threat to the environment and human health. Future research work should focus on estimation of stable O and H isotope compositions of magmatic water related to high-temperature hydrothermal systems in China, which is of significance for the quantitative source study of geothermal fluid recharged by degassed magmatic waters. Attention should also be paid to some constituent species in geothermal fluid of strong environmental significance, such as thioarsenate that is crucial for the fate of As discharged from geothermal springs, especially sulfidic hot springs.

13/01084 Impact of district heating and groundwater heat pump systems on the primary energy needs in urban areas

Verda, V. *et al. Applied Thermal Engineering*, 2012, 40, 18–26.

This work is focused on the planning of rational heating systems for urban areas. From the sustainability viewpoint, district heating is an important option to supply heat to the users in urban areas. The energy convenience of such option depends on the annual energy request, the population density and the efficiency in heat production. Among the alternative technologies, geothermal heat pumps (both open loop and closed loop heat pumps) play a crucial role. This paper aims to propose a procedure to select which users in an urban area should be connected with a district heating network and which ones should be heated through an alternative technology, in order to reach a globally optimal system from the energy viewpoint. The procedure proposes district heating as the initial choice for all the users. The users are then progressively disconnected to the network, according with the primary energy required to supply them heat, and the alternative technology is considered for disconnected users. Here, ground water heat pump is considered as the alternative technology. The total primary energy request is assumed as the objective function to be minimized. To reach this result, the exergetic cost of heat supplied through heat pumps system must be evaluated. Such evaluation is not trivial, as it must include proper analysis of both the district heating network and the alternative system. In the case of densely populated areas, an additional consideration is necessary: the subsurface thermal degradation caused by heat pump installations may affect the performances of surrounding installations. This impact is calculated through a thermo-fluid dynamic model of the subsurface. The application to an Italian town is considered as a test case. The optimal configuration of the overall urban heating system is obtained. This configuration corresponds to the minimum primary energy request to supply heat to all the users (those connected to the network and those using an alternative heating system).

13/01085 Performance analysis of a novel integrated geothermal-based system for multi-generation applications

Ratlamwala, T. A. H. *et al. Applied Thermal Engineering*, 2012, 40, 71–79.

This paper proposes a novel integrated, geothermal-based double flash power generating, ammonia-water quadruple effect absorption, and electrolyser system for cooling, heating, power, hot water and hydrogen production. Detailed energy and exergy analyses are carried out, and the effects of geothermal source temperature, geothermal source mass flow rate, geothermal source pressure, effect of ambient temperature are then studied parametrically. It is found that increasing geothermal source temperature, pressure and mass flow rate results in increasing power and rate of hydrogen produced. The amount of hydrogen produced is found to be increasing from 1.85 to 11.67 kg/day with rise in geothermal source temperature from 440 to 500 K respectively, and from 7.9 to 9.6 kg/day with increase in geothermal source pressure from 3000 to 5000 kPa, respectively. However, increase in geothermal source temperature, pressure, and mass flow rate has negative effects on cooling production. Moreover, a rise in ambient temperature results in better exergetic efficiency of the system.

13/01086 Performance optimization of a hybrid ground source heat pump with the parallel configuration of a ground heat exchanger and a supplemental heat rejecter in the cooling mode

Park, H. *et al. International Journal of Refrigeration*, 2012, 35, (6), 1537–1546.

A hybrid ground source heat pump (HGSHP) combining a ground flow loop and a supplemental heat rejecter loop in parallel is proposed to overcome the degradation of the ground thermal condition. The objective of this study is to optimize the performance of the HGSHP with the parallel configuration by varying the amount of refrigerant charge, the secondary fluid flow rate of the ground loop, and the secondary fluid flow rate of the supplemental loop. The coefficient of performance of the HGSHP with the parallel configuration was 21% higher than that of the conventional ground source heat pump (GSHP), and the heat rejection rate of the ground flow loop was 42% lower than that of the GSHP at the entering fluid temperature (EFT) of 40 °C in the ground heat exchanger and the EFT of 28 °C in the supplemental heat exchanger.

13/01087 QrtzGeotherm: a revised algorithm for quartz solubility geothermometry to estimate geothermal reservoir temperature and vapor fraction with multivariate analytical uncertainty propagation

Verma, M. P. *et al. Computers & Geosciences*, 2012, 48, 316–322.

The quartz solubility geothermometry programmed as two classes, *SiO2TD* and *QrtzGeotherm* in the library, *Geotherm* in VB.NET is an accurate and efficient approach to estimate the deep geothermal reservoir temperature and vapour fraction with multivariate analytical uncertainty propagation. The library *Geotherm* can be implemented in any programming environment including Excel. The calculation of temperature and vapour fraction in the geothermal reservoir of Los Azufres geothermal system is illustrated with considering the analytical uncertainty of enthalpy (2%) and SiO_2 concentration (10%). The average uncertainty in the calculated reservoir temperature is ±18 °C, which is relatively high to understand reservoir processes during the exploitation of the geothermal reservoir. Thus the geochemical analysis of geothermal water is first improvement that must be made to obtain a better understanding of the characteristics of geothermal systems with fluid geochemistry. The algorithm of quartz geothermometry with considering only liquid phase in the geothermal reservoir is conceptually incorrect due to lacking of energy (enthalpy) balance. However, both the algorithms provide same results for the wells, which are fed from a single-phase liquid reservoirs.

13/01088 Thermodynamic evaluation of the Afyon geothermal district heating system by using neural network and neuro-fuzzy

Şahin, A. Ş. and Yazici, H. *Journal of Volcanology and Geothermal Research*, 2012, 233–234, 65–71.

In this study, energy and exergy analysis of the Afyon geothermal district heating system (AGDHS) in Afyon, Turkey using artificial neural network (ANN) and adaptive neuro-fuzzy (ANFIS) methods is carried out. Actual system data in the analysis of the AGDHS are used. The results of ANN are compared with ANFIS in which the same data sets are used. ANN model is slightly better than ANFIS in determining the energy and exergy rates. In addition, new formulations obtained from ANN are presented for the determination of the energy and exergy rates of the AGDHS. The R^2-values obtained when unknown data were used in the networks were 0.999999847 and 0.99999997 for the energy and exergy rates respectively, which are very satisfactory.

Solar energy

13/01089 A practical superhydrophilic self cleaning and antireflective surface for outdoor photovoltaic applications

Son, J. *et al. Solar Energy Materials and Solar Cells*, 2012, 98, 46–51.

Much attention has been recently focused on realizing, by chemical treatment, an artificial superhydrophobic surface with elevated roughness in order to achieve both self-cleaning and antireflective effects because superhydrophobic surface with surface functionalization is believed to be effective for the self-cleaning effect, mimicking a lotus leaf. Various hydrophobic, hydrophilic, superhydrophobic, and superhydrophilic glasses are evaluated by monitoring the variation of water contact angle, optical transmittance, and photovoltaic performance under outdoor conditions for 12 weeks. The results show a nanopatterned superhydrophilic glass without surface chemical treatment exhibits more efficient self-cleaning and antireflective effects, leading to only 1.39% of drop of solar cell efficiency during an outdoor test for 12 weeks, while the solar cells with bare glass packaging and fluorinated superhydrophobic packaging show 7.79% and 2.62% of efficiency drop, respectively.

13/01090 Conformal coating of titanium suboxide on carbon nanotube networks by atomic layer deposition for inverted organic photovoltaic cells

Jin, S. H. *et al. Carbon*, 2012, 50, (12), 4483–4488.

This study proposes a new strategy for improving the charge selectivity of carbon nanotubes (CNTs) for organic photovoltaic cells (OPVCs). The strategy involves the coating of an ultrathin layer of titanium suboxide (TiO_x) on CNTs by atomic layer deposition (ALD). ALD can facilitate that conformal and uniform coating of TiO_x on CNT networks while preserving their nanoporous structure. The authors used the TiO_x-coated CNT networks as an electron transport layer in inverted OPVCs. TiO_x-coated CNTs can provide electrons with an extremely fast conductive path through CNTs and selectively block the holes by means of the hole-barrier property of the TiO_x in OPVCs. The nanoporous structure of TiO_x-coated CNT networks can improve the device performance of OPVCs due to synergetic effects of the electron selective transport property of TiO_x and the high conductivity of CNTs. In addition, further improvement of device performance can be achieved by adding a hole transport layer (MoO_3) between the active layer and the Au electrode.

13/01091 Design and fabrication of diffusive solar cell window

Chen, R.-T. *et al. Renewable Energy*, 2012, 40, (1), 24–28.

A diffusive solar cell window was designed and fabricated with uniformly distributed nanocomposite particles in a light diffusive plate that was sandwiched between two glass layers. The entire composite construction transfers light radiation to solar cells at the edge of the windows. It is based on a new combination of existing technologies because of it uses mature, mass-produced components – solar cells – as well as nanocomposite particles that are embedded inside the light-guide plate. They are integrated using an inexpensive and widely used method for making building windows. The result is an inexpensive, strong, stable, view quality-preserving solar energy-harvesting window that has no close competition. The diffusive solar cell window does not suffer from aging, and products that are made using diffusive solar cell window technology will be new entries to the solar power generation window market.

13/01092 Effect of incident flow conditions on convective heat transfer from the inclined windward roof of a low-rise building with application to photovoltaic-thermal systems

Karava, P. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2012, 104–106, 428–438.

Steady RANS CFD simulations were used to evaluate convective heat transfer from the roof of a low-rise building immersed in an atmospheric boundary layer for different terrain, with relevance to photovoltaic-thermal (PV/T) systems. Dimensionless correlations for the exterior convective heat transfer coefficient (CHTC), expressed as Nusselt number (Nu), were developed for the windward roof, based on Reynolds number and incident turbulence intensity at eaves height, thereby quantifying the strong influence of incident turbulence on the CHTC. Simulations were also performed for a generic flat plate of the same streamwise length so as to provide further insight into the effects of incident turbulence on the windward roof boundary layer. The CHTC values for the windward roof and, hence, the correlations presented here, for a given terrain, are largely insensitive (less than 5% change) to variations in roof slope (from 20° to 45°) or small changes in wind direction (up to 20° from the normal to the eaves). Mixed convection simulations for conditions with significant buoyancy forces (Richardson numbers from 0.9 to 7) show that the CHTC values can be up to 14% higher than those that are based on forced convection only.

13/01093 Efficiency limiting bulk recombination in multicrystalline silicon solar cells

Michl, B. *et al. Solar Energy Materials and Solar Cells*, 2012, 98, 441–447.

This paper measures, spatially resolved, the efficiency potential of multicrystalline material. The excess carrier lifetime in the bulk affects the open-circuit voltage, the short-circuit current and the fill factor of a solar cell differently as different injection conditions apply. Therefore, the authors measure the bulk lifetime injection-dependent and analyse each *IV*-parameter separately. Furthermore, multicrystalline wafers with laterally varying bulk recombination need a spatially resolved analysis to explore the impact of large grains or dislocation clusters on the efficiency. The crucial information needed is the spatially resolved injection-dependent bulk lifetime. For this purpose, lifetime calibrated photoluminescence imaging was used with a varying generation rate. Measuring a surface passivated wafer after the important high temperature steps of a solar cell process ensures that the bulk recombination that is relevant for the solar cell is reached. Combining this information with a cell simulation, the authors deduced the maximum efficiency for every image point. They also discuss how to obtain global values from these images and investigate the effect of charge currents flowing laterally through the emitter using Sentaurus Device and Spice network simulations. A comparison of these simulated global values to measured *IV*-parameters on finished solar cells shows good agreement between the two. A detailed analysis of two mc-wafers from different feedstock shows limiting *IV*-parameters in different regions, efficiency reductions due to dislocations and explains differences in the fill factor of two equally processed solar cells. The analysis shows that evaluating the material related efficiency limitation of silicon wafers has to be done at the efficiency level, as the lifetime at one generation level alone is not sufficient.

13/01094 Experimental analysis on thermal performance of a solar air collector with a single pass

Yang, M. *et al. Building and Environment*, 2012, 56, 361–369.

Five critical parameters may have influence on the thermal performance of a solar air collector with one pass: (1) heat transfer resistance in the airflow channel, (2) height of the stagnant air layer, (3) optical properties of the transparent cover, (4) emittance of the absorber plate and (5) conductive thermal resistance of the back plate. In order to show the actual effects of these parameters, six collectors, each was made by changing one critical parameter mentioned above, were tested under the same working conditions. Thermal efficiency was employed as the main indicator. Results show that decreasing heat transfer resistance in the airflow channel played the most significant role in improving thermal efficiency. Adjusting the height of the stagnant air layer and improving the optical properties of the transparent cover played the secondary role. Increasing the conductive thermal resistance of the back plate and decreasing the emittance of the absorber plate had the least impact. The results would be useful to guide or optimize solar air collector design.

13/01095 Experimental investigation of extra-long pulsating heat pipe application in solar water heaters

Arab, M. *et al. Experimental Thermal and Fluid Science*, 2012, 42, 6–15.

In this study, the aim is to investigate the application of pulsating heat pipes (PHPs) as a heat transfer tool in a solar water heater (SWH). For this purpose, an extra-long pulsating heat pipe (ELPHP) is designed, constructed and installed in a thermosyphon solar water heater. In this work the ELPHPs are made of copper tubes of internal diameter 2.0 mm. The number of meandering turns is six and the working fluid employed is distilled water. The lengths of condenser and evaporator sections are 0.8 and 0.96 m, respectively. The length of adiabatic section varies between 0.7 and 1.8 m. Inclination of the ELPHPs varies between 15° and 90° but is 45° for evaporator section. Four different tests are carried out; SWH with thermosyphon cycle, SWH with PHP filling ratio (FR) = 30%, FR = 50% and FR = 70%. The results show that PHP with FR = 70% has the most stable and the longest functioning duration. While mean temperature of container water is 35.3 and 34.5 °C for thermosyphon cycle and PHP FR = 70%, respectively, the surface area under the container water temperature curve vs time for thermosyphon is 87.69% of that of PHP FR = 70% which indicates the higher heat transfer rate for the ELPHPs. In addition, calculations show efficiency of PHP FR = 70% is equal to 53.79% while efficiency of thermosyphon mode is in range of 31% and 36%.

13/01096 Experimental study of a photovoltaic solar-assisted heat-pump/heat-pipe system

Fu, H. D. *et al. Applied Thermal Engineering*, 2012, 40, 343–350.

A practical photovoltaic solar-assisted heat-pump/heat-pipe (PV-SAHP/HP) system has been designed and constructed in this study. Experiments were conducted from 1 November to 7 December 2010 under the meteorological conditions of Hong Kong. Based on the test data, the instantaneous and daily performance of the system operating in the heat-pipe and the solar-assisted heat-pump modes was studied using energy and exergy analyses. The results showed that the PV-SAHP/HP system could reach a daily average energy efficiency of 61.1–82.1% and an exergy efficiency of 8.3–9.1% when operating in the solar-assisted heat-pump mode. The daily average heat-pump COP could reach 4.01 when solar radiation was strong. The daily average system energy and exergy efficiencies were approximately 36.5–38.4% and 7.4–7.8%, respectively, when the PV-SAHP/HP system operated in the heat-pipe mode under strong solar radiation. The system energy generation and exergy output factors in this mode reached maximum values of 28.9 and 5.36, respectively. The PV-SAHP/HP system operating in the heat-pipe mode is more significant for energy savings, but the water in the tank could hardly reach the temperature viable for domestic hot water when solar radiation was weak. On the other hand, the system could heat water to the temperature viable for domestic hot water when operating in the solar-assisted heat-pump mode, even when solar radiation was weak. Therefore, the PV-SAHP/HP system provides the optimal operating modes for energy savings and actual demand.

13/01097 Finite element method simulations of heat flow in fixed bed solar water splitting redox reactors

Bulfin, B. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10028–10035.

An improved design for radiation absorption and heat flow into materials with low thermal conductivity is demonstrated. The design was developed for application in fixed bed two-step solar water splitting redox reactors. The fixed bed was assumed to be made from porous ceramic. The low thermal conductivity of the porous ceramic redox material is compensated for by changing the profile of the fixed bed. The profiling used was wedges cut into the material which allows concentrated solar radiation to be incident on a larger area of redox material than for a flat monolith design. The design is demonstrated to efficiently transfer heat to the bulk and greatly reduce re-radiation. For a wedge 9 cm in depth and 1.6 cm wide at the opening, heated with $500\,\mathrm{kW\,m^{-2}}$ incident radiation for 300 s, approximately double the amount of radiation is absorbed. The effects of thermal conductivity, emissivity and scaling on the efficiency of the design were investigated. The radiation absorption performance improved when scaled up. The improvement of the design over a flat plain bed is greater for lower emissivity. The improvement provided by the wedge design was found to decrease for increasing thermal conductivity, and eventually for high conductivity values it reduced performance. Using this method a larger amount of material with low thermal conductivity can be heated with the same power input and reduced radiation losses. The heat flow simulations were then coupled to an Arrhenius rate equation to investigate the possible improvement to the reaction efficiency and yield offered by the wedge design. Over a time of 300 s the efficiency and yield were seen to be approximately a factor of four times higher in the wedge case. Finally a concentrated solar cavity reactor based on the design is proposed.

13/01098 Influence of Sn doping on ZnO nanostructures from nanoparticles to spindle shape and their photoelectrochemical properties for dye sensitized solar cells

Ameen, S. *et al. Chemical Engineering Journal*, 2012, 187, 351–356.

Tin (Sn)-doped zinc oxide (ZnO) nanostructures were synthesized by a simple hydrothermal method and the photovoltaic performances of Sn-doped ZnO-derived photoanodes were studied. The doping of Sn significantly altered the morphology of ZnO into spindle shape by the arrangement of small ZnO nanoparticles. The crystalline and structural properties deduced the clear decrement in the crystallite sizes from ∼143.9 to ∼82.2 nm, which might be suggested the doping of Sn-ions into ZnO nanostructures. X-ray photoelectron spectroscopy (XPS) study showed Sn–O and Zn–O bonding in the synthesized spindle shaped Sn-ion doped ZnO nanostructures, which confirmed the Zn substitution by the Sn-ions. Dye sensitized solar cell (DSSC) fabricated with Sn-ZnO photoanode achieved a solar-to-electricity conversion efficiency of ∼1.82% with short circuit current (J_{SC}) of $5.1\,\mathrm{mA/cm^2}$, open circuit voltage (V_{OC}) of 0.786 V and fill factor (FF) of 0.45, which was higher than that of DSSC with ZnO photoanode. The increased conversion efficiency and the photocurrent density were attributed to the significant Sn-ion doping into ZnO nanostructures and considerable arrangement of ZnO nanoparticles into spindle shaped morphology which might improve the high charge collection and the transfer of electrons at the interfaces of doped ZnO layer and the electrolyte layer.

13/01099 Modeling of a two-step solar hydrogen production plant

de la Calle, A. *et al. International Journal of Hydrogen Energy*, 2012, 37, (14), 10549–10556.

The promising advances in research in two-step solar hydrogen production from water have increased interest in producing hydrogen with this technology. In this framework, the Hydrosol II Project pilot plant for producing continuous solar hydrogen from water using a ferrite-based redox technology was erected at the CIEMAT-Plataforma Solar de Almería. Two reactors allow the oxidation and reduction steps to be performed in parallel, which, sequentially switched, make hydrogen production quasi-continuous. A dynamic model of a solar hydrogen production plant has been developed based on experience with this pilot plant. As it was designed as a control algorithm test platform, for practical control issues, some simplifications have been assumed to make the model suitable. The new model includes both a solar field model and a processing plant model and is able to simulate the concentrated solar power received by the reactors and the thermal and chemical reactor behaviour. The solar field model and plant thermal behaviour were calibrated and validated with experimental data. The numerical predictions show good agreement with measurement data.

13/01100 Monthly average daily global solar irradiation maps for Uganda: a location in the equatorial region

Mubiru, J. *et al. Renewable Energy*, 2012, 41, 412–415.

Proper sizing of solar energy systems is necessary in order to optimize their output. This requires a database of solar irradiation for locations for which the systems are being assessed. Solar irradiation data is also required in modelling a building's thermal performance, as input into ecological and crop models and evaluation of long-term effects of climatological changes. Solar irradiation data can be provided through measurements. In Uganda, measurements of global solar irradiation have been carried out for a few locations because the measuring instruments are expensive to purchase and install. An alternative to obtaining solar irradiation data is to estimate it either by use of an appropriate solar irradiation model or interpolation of the few existing records. The present study attempted to draw global solar irradiation maps for Uganda. Global solar irradiation values were estimated for eight out of twelve stations using an artificial neural networks model proposed for Uganda. Measured values of monthly average daily global solar irradiation were used for the remaining four stations. The values for the 12 stations were then utilized for the interpolation using moving average method. The result is a set of 12 global solar irradiation maps for Uganda with relative errors in the range of 8–16%.

13/01101 Net energy analysis for concentrated solar power plants in northern Chile

Larraín, T. and Escobar, R. *Renewable Energy*, 2012, 41, 123–133.

Chilean energy policy goals attempts to promote efficiency and sustainability in the energy system. These objectives have been considered in recent modifications to the electricity generation laws by establishing that generation companies must reach a quota of up to a 10% from renewable energy sources by 2024. Concentrated solar power (CSP) is an interesting alternative to help achieve those objectives, as it is estimated that northern Chile has high radiation levels, coupled with the high values of the local clearness index and flat land availability. However, from the sustainability point of view it seems necessary to assess if a CSP plant is effectively an energy source. Here the authors propose a hybrid solar power plant lifecycle model which through a net energy analysis obtains and analyses the plant energy sustainability attributes such as net energy, energy return over investment and energy payback time. The stages of construction, operation, maintenance and decommissioning are considered in the lifecycle analysis. The model is then applied in order to determine good locations where to install a CSP plant in the Chilean Atacama desert. Monthly means of solar radiation are used in order to estimate the solar fraction for a 100-MW direct steam generation parabolic trough collector plant. The results indicate that solar power plants are effectively a net energy source for the analysed locations, and that higher energy costs are related to the fossil fuel backup lifecycle. A relation is established between yearly radiation, energy return over investment and energy payback time. It is estimated that the net energy analysis is a useful tool for determining under which conditions a power plant becomes a net energy source and therefore a more convenient option from the sustainability point of view, and thus can be utilized in order to define best geographical locations and operation conditions for different renewable energy sources. The sustainability attributes are greatly enhanced when considering a solar-only operation mode, which highlights the advantages of using that configuration, and presents a case for the use of thermal energy storage systems rather than fossil-fuel hybridization if a constant or dispatchable energy profile is required.

13/01102 Numerical study on combined free-forced convection heat loss of solar cavity receiver under wind environments

Xiao, L. *et al. International Journal of Thermal Sciences*, 2012, 60, 182–194.

A numerical study has been carried out to investigate the impact of wind on combined free-forced convection loss from a fully open solar cavity receiver for high-temperature dish/engine system. Visualization results, i.e. velocity vector field, temperature and velocity contours are provided to reveal the wind effect. The variations of combined free-forced convection heat loss with wind speed, wind incidence angle as well as the receiver inclinations have been quantitatively analysed. Results show that, the combined convection heat loss for some wind cases may not decrease monotonically with increasing inclinations as that of no-wind cases. Under some certain wind conditions, the combined convection heat loss may possibly be reduced below the natural convection value, and there exists critical wind speed that minimizes the combined convection heat loss. Moreover, the combined convection heat loss of receiver at different inclinations becomes more and more indistinguishable as wind speed increases. Finally, a simple correlation has been proposed to estimate the convection heat loss variation caused by the environmental wind.

13/01103 Optimization of the electronic driver and thermal management of LEDs lighting powered by solar PV

Fathi, M. *et al. Energy Procedia*, 2012, 18, 291–299.

The development of efficient photovoltaic (PV) standalone systems requires advanced technology for PV cells and modules for high performance but also the application of components or loads of use with low-energy consumption. In this context, the development of lighting systems using solar energy and electroluminescent components like high power white light-emitting diodes (LEDs) is proposed. The integration of the light fixture with the choice of best technologies for high-efficiency LEDs and the design of an ultra-economic driver as the PWM driver permit us to obtain a high lighting efficiency. This study has taken in consideration thermal aspect and the choice of adequate heat sinks for thermal management. The study considered both effects of thermal and electronic order and the achievement of a high-efficiency lighting powered by solar energy. With the implementation of the PWM electronic controls, an energy efficiency of the LEDs driver should increase from 85 to 90%.

13/01104 Performance evaluation of eight contemporary passive solar homes in subtropical Australia

Miller, W. *et al. Building and Environment*, 2012, 56, 57–68.

Subtropical south-east Queensland's expanding population is expected to lead to a demand for an additional 754,000 dwellings by 2031. A legacy of poor housing design, minimal building regulations, an absence of building performance evaluation and various social and market factors has led to a high and growing penetration of, and reliance on, air-conditioners to provide comfort in this relatively benign climate. This reliance impacts on policy goals to adapt to and mitigate against global warming, electricity infrastructure investment and household resilience. Based on the concept of bioclimatic design, this field study scrutinizes eight non-air conditioned homes to develop a deeper understanding of the role of contemporary passive solar architecture in the delivery of thermally comfortable and resilient homes in the subtropics. These homes were found to provide inhabitants with an acceptable level of thermal comfort (18–28 °C) for 77–97% of the year. Family expectations and experiences of comfort, and the various design strategies utilized were compared against the measured performance outcomes. This comparison revealed issues that limited quantification and implementation of design intent and highlighted factors that constrained system optimization.

13/01105 State-of-the-art building integrated photovoltaics

Jelle, B. P. and Breivik, C. *Energy Procedia*, 2012, 20, 68–77.

Building integrated photovoltaic (BIPV) systems may represent a powerful and versatile tool for achieving the ever increasing demand for zero energy and zero emission buildings of the near future. In this respect, BIPVs offer an aesthetical, economical and technical solution to integrate solar cells harvesting solar radiation to produce electricity within the climate envelopes of buildings. This work summarizes the current state of the art of BIPVs, including both BIPV foil, tile, module and solar cell glazing products.

13/01106 Study of the electrical characteristics of poly(o-toluidine) and application in solar cell

Ziadan, K. M. *et al. Energy Procedia*, 2012, 18, 157–164.

Substituted poly(o-toluidine) (POT) was synthesized by a chemical polymerization method using ammonium persulfate as an oxidizing agent. Thin films of POT have been prepared by the spin-coating method and characterized by Fourier transform infrared spectroscopy and atomic force microscopy. The current–voltage characteristic of AL/POT/AL sample at different temperatures (273–383) K was investigated. Ohmic behaviour is shown at all applied voltages. The electrical conductivity increases with increasing temperature from 1.49×10^{-7} S/cm at 293 K to 6×10^{-6} S/cm at a temperature of 383 K. This behaviour indicates that the POT polymer behaves as semiconductor material. The electrical conductivity as a function of reciprocal absolute temperature ($1/T$) was also investigated. The activation energy was determined from the curve as about 0.313 eV. The POT/n-Si solar cells obtained in this work have yielded a conversion efficiency is about 0.88%.

13/01107 Thermophotovoltaic power conversion from a heat-recirculating micro-emitter

Park, J. H. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4878–4885.

Power generation using a novel configuration of a 1–10 W micro-thermophotovoltaic (micro-TPV) device is studied experimentally. A micro-emitter as a thermal heat source is a simple cylinder with an annular-type shield that applies a heat-recirculation concept and an expanded exhaust outlet that facilitates ignition, which provides stable burning in the small confinement and uniform distribution of temperature along the wall. The micro-emitter is surrounded by a chamber with cooling fins, the inner wall of which has an installation of gallium antimonide photovoltaic cells (PVCs). The performance of the micro-TPV device is most favourable at reduced length of the cooling fins unless the temperature on the PVCs is higher than the operating limit temperature for the GaSb cells. The relative position of the micro-emitter to the PVCs also affects the performance of the micro-TPV device. These observations imply that the net amount of heat irradiation onto the PVCs is more dominant than the PVC temperature in determining the TPV performance. Under optimized operating conditions, the micro-TPV device produces 2. W with an overall efficiency of 2.1%, indicating that the efficiency up to the PVC surface is 21% at least if a PVC efficiency of 10% at most is assumed.

13/01108 Using inverse analysis to find optimum nano-scale radiative surface patterns to enhance solar cell performance

Hajimirza, S. *et al. International Journal of Thermal Sciences*, 2012, 62, 93–102.

Nano-scale surface patterning can provide highly spectral-directional absorption properties for thin film solar cells. Achieving optimal surface patterning is an inverse optimization problem that requires a numerical procedure capable of scrutinizing the space of geometry parameters to search for an optimal solution. In this paper, two- and three-dimensional thin film amorphous silicon (a-Si) solar cells with periodic structures are considered, whereby the surface of the solar cell is textured with rectangular metallic nano-patterns for enhancing the solar absorption spectrum. The authors use FDTD simulations to solve Maxwell's equations inside the cell area when subject to standard optical irradiation. By means of several numerical optimization techniques such as the quasi-Newton BFGS method, random search simulated annealing, and Tabu search, they determine optimal specifications for surface nano-patterns. Invoking constrained optimization tools, the authors incorporate various types of practical constraints into the optimization programs. The resulting cell structures found by the inverse solvers illustrate enhancement factors as high as 1.52 in solar absorption when silver nano-patterns are used, compared to bare a-Si cells. Results demonstrate the efficiency of the selected optimization techniques and their computational efficiency in contrast with the naïve brute force alternative and provide a benchmark for comparing the performances of various local and global optimization methods. The global random search optimization techniques (simulated annealing and Tabu search) tend to perform better than the local method (quasi-Newton), especially for higher problem dimensions.

Wind energy

13/01109 A coupled aeroelastic damage progression model for wind turbine blades

Cárdenas, D. *et al. Composite Structures*, 2012, 94, (10), 3072–3081.

The prediction of damage progression in composite wind turbine blades, especially under dynamic aeroelastic conditions, is usually a cumbersome multi-step process with significant manual user intervention. In this paper a novel approach is presented where the different components of this process – dynamical structural analysis under varying aerodynamic and deterministic loads, and damage progression – are integrated into one reduced-order model capable of predicting the occurrence and progression of damage in real time. Key to this integration is the use of an effective one-dimensional model of the turbine blade known as thin-wall beam model, which allows for the reconstruction of a three-dimensional stress field of a volume given by the blade. This stress field can then be used to assess damage and locally modify the structural properties to account for the presence of damage, leading to a reduced load carrying capacity. The model was previously tested in its components, demonstrating a good agreement of the predicted structural and static damage progression behaviour compared to detailed high-order finite-element models of the same blade. Once validated, the model was applied to severe load cases and the potential for real-time predictions of damage progression was demonstrated.

13/01110 Aggregated models and transient performances of a mixed wind farm with different wind turbine generator systems

Li, H. *et al. Electric Power Systems Research*, 2012, 92, 1–10.

This paper proposes a genetic algorithm (GA)-based method for the aggregation of a mixed wind farm with different wind turbine generator system (WTGS) parameters, and discusses the transient performances of a grid-connected wind farm with a squirrel-cage induction generator (SCIG) and a doubly fed induction generator (DFIG). First, the transient models of a SCIG-based WTGS and DFIG-based WTGS are presented. Then, by using the GA to minimize the error of the output power between the aggregated single-generator model and the investigated wind farm, an aggregate method for a mixed farm is proposed and validated. The proposed method is shown to be superior to the traditional method with respect to the aggregation of a mixed wind farm in terms of different WTGS parameters. Finally, the transient performances of a mixed wind farm, including the output active power and the output voltage, are investigated by using the proposed method. The simulation results show that the transient behaviours of the mixed wind farm are closely related to the generator capacity ratio, the short-circuit capacity (SCC) ratio and the impedance ratio of the connected power system.

13/01111 Conversion of squirrel cage induction motors to wind turbine PMG

Farooqui, S. Z. *Renewable Energy*, 2012, 41, 345–349.

A relatively simple and low cost method for making permanent magnet wind turbine electric generators from burnt out squirrel cage induction motors, has been described in this paper. Different types of generators used in wind turbines and the general properties sought in a wind turbine generator are discussed first, and then the procedure of how to make a workable, multi-pole, low speed, permanent magnet generator (PMG), from burnt out ordinary squirrel cage induction motors easily available at through away prices in the junk markets, is described. Finally, the test results of a 500 and a 1500 W generator developed this way are presented with their cost and performance analysis.

13/01112 Cost reductions for offshore wind power: exploring the balance between scaling, learning and R&D

van der Zwaan, B. *et al. Renewable Energy*, 2012, 41, 389–393.

Offshore wind electricity generation is prospected to increase substantially in the near future at a number of locations, like in the Baltic, Irish and North Sea, and emerge at several others. The global growth of offshore wind technology is likely to be accompanied by reductions in wind park construction costs, both as a result of scaling and learning effects. Since 2005, however, significant cost increases have been observed. A recent surge in commodity prices proves to constitute one of the main drivers of these cost increases. This observation begs the question whether wind turbine manufacturers should return to the laboratory for undertaking R&D that explores the use of alternative materials and bring offshore wind energy closer to competitiveness. It is demonstrated that if one abstracts from material price fluctuations, in particular for metals such as copper and steel, turbine production plus installation cost data publicly available for a series of offshore wind park projects (realized in several European countries since the 1990s) show a cost reduction trend. Hence various other sources of cost increases, such as due to the progressively larger distances from the shore (and correspondingly greater depths at sea) at which wind parks have been (and will be) built, are outshadowed by cost reduction effects. When one expresses the overall cost development for offshore wind energy capacity as an experience curve, a learning rate is found of 3%, which reflects a mixture of economies-of-scale and learning-by-doing mechanisms. Also the impact is quantified on offshore wind power construction costs from the recent tightness in the market for turbine manufacturing and installation services: without the demand-supply response inertia at the origin of this tightness it is estimated that the learning rate would be 5%. Since these learning rates are relatively low – in comparison to those observed for other technologies, and in view of the high current capacity costs of offshore wind in comparison to onshore wind energy – a renewed focus on learning-by-searching or R&D is recommended.

13/01113 Current facts about offshore wind farms

Madariaga, A. *et al. Renewable and Sustainable Energy Reviews*, 2012, 16, (5), 3105–3116.

This paper reviews offshore wind projects with a wide perspective. The current situation of the offshore wind market is presented, pointing out the countries leading the process in terms of installed capacity and in terms of technological leadership. Feasibility studies of alternative offshore wind farms are interesting not only in relation to the business but in relation to the technoeconomic analyses that engineering researchers need to do. Details about the average energy yield assessment, the costs and the price for the purchased energy are commented on, as key elements of those feasibility studies. The higher cost of renewable energy sources of electricity when compared with conventional sources, demands appropriate policy support. The European regulatory framework and the support schemes established by European Union member states are presented, as well as the role that different transmission system operators are playing at the moment. Finally, most of the offshore wind farms currently operating are presented, analysing the technical characteristics of their electric subsystems: the wind energy conversion systems transforming the kinetic energy of the wind into electricity, the collector system gathering the power output of all the turbines to a central collection point and the transmission system taking that power to the onshore main grid.

13/01114 Development of small wind turbines for moving vehicles: effects of flanged diffusers on rotor performance

Chen, T. Y. *et al. Experimental Thermal and Fluid Science*, 2012, 42, 136–142.

The main object of this research is to develop a shrouded, small, horizontal-axis wind turbine for moving vehicles. Specifically, this study investigates the effects of flanged diffusers on rotor performance of small (30 cm rotor diameter) wind turbines with different rotor solidities (20–60%) and wind speeds (10–20 m/s). The experiments are conducted in a wind tunnel with and without a flanged diffuser. Results show that the flanged diffuser may significantly increase the power output, torque output, and rotor rotational speed of the wind turbine, largely depending on rotor solidity and wind speed. The higher the solidity and wind speed are, the smaller the effect of the flanged diffuser is. The 30%- and 40%-solidity rotors generate the largest power and torque outputs, respectively, while the 60%-solidity rotor has the lowest rotor rotational speed among the test rotors. These results provide some useful information when considering rotor-generator matching problems and the selection of rotor solidity for moving vehicles. This study also shows that a small wind turbine has the characteristics of low torque and high rotor rotational speed, and high rotor solidity for maximum power output compared to a conventional large wind turbine.

13/01115 Dynamic model of wind energy conversion systems with PMSG-based variable-speed wind turbines for power system studies

Sanchez, A. G. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10064–10069.

In order to study the impact of a wind farm on the dynamics of the power system, a significant issue is to develop appropriate equivalent models that allow characterizing the dynamics of all individual wind turbine generators (WTGs) composing the park. In this sense, with the advance of power electronics, direct-driven permanent magnet synchronous generators (PMSGs) have drawn increased interest to wind turbine manufacturers due to their advantages over other variable-speed WTGs. These include the possibility of multi-pole design with a gearless construction that offers slow speed operation and reduced maintenance since no brushes are used, elimination of the excitation system, full controllability for maximum wind power extraction and grid interface, and easiness in accomplishing fault-ride through and grid support. In this way, this paper presents a comprehensive dynamic equivalent model of a wind farm with direct-driven PMSG wind turbines using full-scale converters and its control scheme. The proposed simplified modelling is developed using the state-space averaging technique and is implemented in the MATLAB/Simulink environment. The dynamic performance of the wind farm and its impact on the power system operation is evaluated using the phasor simulation method.

13/01116 Effect of drag on the performance for an efficient wind turbine blade design

Almukhtar, A. H. *Energy Procedia*, 2012, 18, 404–415.

The utilization of wind energy for power generation purposes is becoming increasingly attractive and gaining a great share in the electrical power production market worldwide. In the present study, a mathematical model is developed to study the parameters that affect the electrical power generated by the wind turbines. The considered parameters are turbine swept area, air density, wind speed, lift/drag ratio and power coefficient as a function of blade tip speed. The study shows that the operational aerodynamic parameters has a direct effect on the generated power which will lead the developers and researchers to focus on the highest aerodynamics priority that should be considered for manufacturing and suitable the new generations of wind turbines.

13/01117 Gust-front loading effects on wind turbine tower systems

Kwon, D. K. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2012, 104–106, 109–115.

With an increasing focus on the issues of extreme wind events, particularly thunderstorms and downbursts, it is important not to lose sight of their impact with regards to other industrial structures, which are themselves sensitive even to typical flow fields. For the treatment of conventional boundary layer winds, a gust loading factor approach has been widely adapted in most international codes and standards for the design of buildings. Wind turbine towers, though fundamentally different from buildings when viewed as a multi-body system featuring a tower/nacelle and blades, may be treated much in the same way with modified gust loading factors. This paper introduces a possible approach to mesh conventional treatments of gust loading factors with those of newly introduced gust-front factors on wind turbine towers. Much like gust-front factors for buildings, this approach encapsulates many of the varied kinematic and dynamic changes associated with non-stationary characteristics of gust-fronts originating from thunderstorms/downbursts and the changing aerodynamics on wind turbine towers. From an example of a wind turbine tower system, gust-front loading effects as compared to those of boundary layer winds are investigated.

13/01118 Modeling and simulation of windgenerator with fixed speed wind turbine under Matlab-Simulink

Saheb-Koussa, D. *et al. Energy Procedia*, 2012, 18, 701–708.

The rapidly growing wind industry is displaying the need for education and training worldwide, particularly on the system level. Modelling and simulating wind generator systems using Matlab-Simulink provides expert help in understanding wind systems engineering and system design. Working under Matlab-Simulink, this paper presents the integration of the developed WECS model with public electrical grid. A test of the calculated power and C_p related to the experimental equivalent data, using statistical analysis is performed. The statistical indicators of accuracy show better results of the presented method with RMSE: 21%, 22%, MBE: 0.77%, 0.12% and MAE: 3%, 4%. To study its behaviour when integrated in whole power system, three levels of wind speeds were chosen: low with 5 m/s as the mean value, medium with 8 m/s as the mean value and high speed with 12 m/s as the mean value. These allowed predicting and supervising the active power produced by the system, characterized respectively by the middle powers of −150, −250 and −480 kW which will be injected directly into the public electrical grid and the reactive power, characterized respectively by the middle powers of 60, 180 and 320 kW and will be consumed by the wind generator.

13/01119 Multivariable 2-sliding mode control for a wind energy system based on a double fed induction generator

Evangelista, C. A. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 10070–10075.

The purpose of this paper is to present a control strategy using multiple input/multiple output (MIMO) second-order sliding modes (SOSM) for a grid-connected variable-speed wind energy conversion system (WECS). The latter is based on a double-fed induction generator (DFIG) in a bidirectional configuration with slip power recovery. Its points of operation can be electronically controlled and, with them, two independent control objectives can be stated. Thus, a control is designed to maximize the energy captured from the wind and to regulate the stator reactive power, contributing to the compensation of the power factor according to grid requirements. The proposed technique can be applied to non-linear MIMO systems and allows a separate design for each component of the controller. For these designs the super-twisting algorithm is employed in this work, which possesses excellent properties regarding simplicity of implementation and online operation, and robustness against uncertainties and external disturbances. To determine the bounding design constants, the system was thoroughly analysed and simulated during the off-line tuning procedure, considering realistic operating conditions and several bounded disturbances. The reduction of mechanical efforts and chattering were prioritized when fine-tuning the controller. It should be pointed out that while the determination of the bounds is carried out off-line, the control law is rather simple and it can be easily implemented, therefore it operates online with low computational burden. Finally, simulations of the controlled system operating in the partial load zone, under realistic working conditions, showed the achievement of both control objectives and the robustness against external disturbances and variations of the parameters of the models with respect to their rated values.

13/01120 Optimal reactive power allocation in an offshore wind farms with LCC-HVdc link connection

Montilla-DJesus, M. *et al. Renewable Energy*, 2012, 40, (1), 157–166.

This paper addresses the optimal operation of an offshore wind farms (OWF), consisting of 120 wind turbines with doubly fed induction generators (DFIG) and a high-voltage dc (HVdc) connection with the grid, using line commutated converters (LCC). For an optimal operation of the OWF, the distribution of the reactive power set points throughout the wind turbine generators must be optimal, in order to achieve minimum losses within the wind farm and the HVdc transmission system and therefore obtain the maximum production output. To accomplish this objective, an optimization formulation has been proposed which includes a complete model of the OWF and the LCC-HVdc, and the study of two different configurations. Simulation results show the advantages of using the reactive capability of the DFIG to achieve the optimal operation of the OWF.

13/01121 Reality and prospects of wind power in Syria

Amer, En. R. and Hamed, F. A. *Energy Procedia*, 2012, 19, 55–62.

Every day Syria needs SYP500 million as a fuel cost for electric generation stations, which is equal to SYP170 billion per year. There are 5.3 million subscribers, each of them receives annual subsidies of US$320. In order to avoid expected shortage of electric energy this year and for following years, a contract has been concluded with Turkey to provide Syria with 550 MW. Notably, there are many projects under construction now, which will support the electricity net by 2600 MW nearly. Theoretical wind potential in Syria is estimated by 80,000 MW. By primary evaluation of promising areas, it was found that the actual wind potential is close to theoretical one. Currently, installing wind surveillance stations is increasing in the promising areas gradually by installing 25 stations. There are many projects under construction in different Syrian areas. It is expected that wind farms could provide the electricity net with approximately 150 million kWh.

13/01122 Thermal analysis of wind turbine nacelle operating in Algerian Saharan climate

Smaili, A. *et al. Energy Procedia*, 2012, 18, 187–196.

Wind turbines installed in Saharan climate operate often under severe weather conditions. Particularly, the electric/electronic equipment located within the nacelle may be subjected to extremely high temperature. To maintain acceptable temperature levels inside the nacelle and control efficiently the thermal effect, cooling systems should be used properly. This paper presents a numerical method to investigate the nacelle thermal behaviour of wind turbines operating under extremely hot weather conditions. The air flow in and around nacelle is described through the Reynolds averaged Navier–Stokes equations. The energy equation has been used to account for heat transfer effects. A control-volume finite element method has been used to solve the resulting governing equations. The simulations have been performed through a typical commercial wind turbine. Results including temperature fields in and around the nacelle have been obtained and showed quite reasonable behaviour. Mainly, the impact of an appropriate cooling system that can be designed and applied in nacelle thermal control is presented and discussed.

13/01123 Voltage regulation capability of a prototype static VAr compensator for wind applications

Boynuegri, A. R. *et al. Applied Energy*, 2012, 93, 422–431.

Power quality of distribution networks is severely affected with the increasing of wind penetration in power systems. One of the most important considerations in grid integration of wind energy is voltage variations. This paper presents a prototype static VAr compensator

(SVC) that considers RMS value of grid voltage power as reference for reactive power regulation of wind turbines in order to decrease voltage fluctuations. The simulation and experimental studies have demonstrated the effective influences of the SVC on the voltage profile, even in the case of the sudden changes in the voltage magnitude. Furthermore, the experimental results give fairly good agreements with the simulation results.

Others, including economics

13/01124 A 10 year installation program for wave energy in Ireland: a case study sensitivity analysis on financial returns

Dalton, G. J. *et al. Renewable Energy*, 2012, 40, (1), 80–89.

This paper is a case study which examines the finances of a proposed installation schedule of 500 MW of a wave energy device type in Ireland. The novel aspects of the analysis were the modelling of the combined influence of learning curves, supply and demand rates as well as future cost of cash on the phased deployment over 10 years. There are many studies which have examined the economics of renewable energy project installations, including wave energy. However, there is lack of research in the impact and implications of phased installations over time, especially when using a feed-in tariff (FIT) revenue mechanism. The goal of the study was twofold. The first goal was to assess the viability of the current Irish feed-in tariff within the context of a phased installation program for the wave energy device chosen for the study, and measures required to produce a positive rate of return. The second aim was to assess the impact of learning curve, supply/demand curves and future cost of cash on phased project installations. The wave energy device chosen for the study was the Pelamis P1 and the economic model used was NAVITAS, created by HMRC. The assessment was based on net present value and internal rate of return. The wave energy data for the study was 2007 from M4 of the west coast of Ireland, obtained from Marine Institute, Ireland. Results from the case study indicated that the high initial costs for the case study wave energy device had a significant impact on financial returns. Results of the case study indicate that higher tariffs may be required than the current Irish, static, non-index linked, FIT to foster positive returns for future wave energy projects, especially if phased installations are considered, which are susceptible to future cash and supply/demand factors. The large range of sensitivity factors assessed in the case study demonstrates the vulnerable nature of these large scale projects when estimating financial returns. Further studies will be required to assess multiple device types, update initial costs for wave energy devices, provide reliable power matrices, as well as appropriate learning curve and supply demand rates.

13/01125 A new perspective in optimum sizing of hybrid renewable energy systems: consideration of component performance degradation issue

Erdinc, O. and Uzunoglu, M. *International Journal of Hydrogen Energy*, 2012, 37, (14), 10479–10488.

The ever-increasing demand for energy and the concerns on the environmental sustainability issue all around the world lead to more interest in alternative sources for energy production. However, as the current costs of the alternative sources such as solar, wind energy conversion systems etc. are relatively higher as compared to the conventional means of energy production, an optimum sizing approach is quite necessary in order to avoid over-sizing of such systems without lowering the reliability of load demand supply in all possible conditions including the variability of meteorological conditions or the changing power demand of load. There are many research papers available in the literature dealing with this optimum sizing issue. Even the mentioned papers significantly contribute to the wider penetration of such sources, none of them consider the power output degradation of alternative energy sources due to aging during their pre-defined operating life time. Besides, there are a few studies utilizing detailed dynamic models of energy sources apart from first-degree linear equations based models that may fall short in presenting the exact dynamics of the related system. Thus, an ‘observe and focus’ algorithm based optimization of a hybrid alternative energy system considering the power output degradation and detailed models of each hybrid system component is performed in this study. Related details presented within the paper can provide a new perspective in optimum sizing of such hybrid systems and may further be considered in future updates of famous sizing software programs commercially or freely available in websites of several laboratories or universities.

13/01126 Characterization of green roof components: measurements of thermal and hydrological properties

Ouldboukhitine, S. E. *et al. Building and Environment*, 2012, 56, 78–85.

In this study, three of the main physical properties of green roofs were experimentally investigated to determine some of the key green roof modelling parameters. First, the thermo-physical properties of green roofs were characterized by correlating the thermal conductivity of the substrate with the water content for different substrates and maximum water capacities. Next, the moisture storage was characterized using the dynamic vapour sorption technique to determine both the sorption and desorption isotherms for three different temperatures as well as the moisture buffer capacity. Third, the micro-structural properties of green roof substrate were characterized using mercury intrusion porosimetry to measure the porosity range of the substrate and to compare this porosity range with different concrete porosities. In addition to these characterizations, the evapotranspiration term, which is very important in the water balance, was measured. The few studies found in literature provide the expression of the evapotranspiration term for a watered grass and vegetated areas on a large scale. In this study, this term is expressed for the experimentally studied green roof complex (substrate + vegetation). The ultimate objective of these experiments is to estimate the parameters used as input data in the developed green roof model to evaluate the energy performance of a building.

13/01127 Deterministic optimal management strategy of hydroelectric power plant

Bensalem, A. *et al. Energy Procedia*, 2012, 18, 225–234.

This paper makes a comparison between two management strategies of hydroelectric power plan consisting of multi-reservoirs. The first strategy is based on the maximization of the reservoir contents at the end of the exploitation horizon. The second strategy is based on the maximization of the reservoir contents at the end of the sub-periods of the same exploitation horizon. To solve such problem, the authors propose a new objective function model which permits to minimize the use of water. This model is based on the enhancement of the water value in function of its location in any reservoirs of the system and of the waterfall height. Hence, the objective function is represented in function of the water potential energy stored in all reservoirs.

13/01128 Developing a model for assessing biomass processing technologies within a local biomass processing depot

Bals, B. D. and Dale, B. E. *Bioresource Technology*, 2012, 106, 161–169.

One solution to the supply chain challenges of cellulosic biofuels is a network of local biomass processing depots (LBPDs) that can produce stable, dense, intermediate commodities and valuable co-products prior to shipping to a refinery. A techno-economic model of an LBPD facility that could incorporate multiple technologies and products was developed in Microsoft Excel to be used to economically and environmentally evaluate potential LBPD systems. In this study, three technologies (ammonia fibre expansion or AFEX^{TM} pretreatment, fast pyrolysis, and leaf protein processing) were assessed for profitability. Pyrolysis was slightly profitable under the base conditions, leaf protein processing was highly unprofitable, and AFEX was profitable if biomass drying was not required. This model can be adapted to multiple feedstocks and end uses, including both economic and environmental modelling.

13/01129 Energy security and hydropower development in Malaysia: the drivers and challenges facing the Sarawak corridor of renewable energy (SCORE)

Sovacool, B. K. and Bulan, L. C. *Renewable Energy*, 2012, 40, (1), 113–129.

This article investigates the drivers and challenges associated with the Sarawak corridor of renewable energy (SCORE) in Malaysia on the island of Borneo. SCORE constitutes a multi-hundred billion dollar infrastructure development plan in Sarawak, one aiming to achieve US$105 billion of investment and to build 20,000 MW of hydroelectric dams along a 320 km corridor criss-crossing 70,000 km^2. Based largely on primary data collected through site visits, original field research in Sarawak, and more than 80 research interviews, this paper identifies the genesis of SCORE, its expected benefits, and challenges with implementation encountered to date. The article begins by describing its research methods and then summarizes four sets of anticipated benefits discussed by respondents associated with SCORE: industrialization, energy security, equitable development, and spillover effects. It then dives into a longer discussion of the technical, economic, political, legal and regulatory, social, and environmental challenges facing the project. The article concludes by offering implications for those wishing to promote other large-scale, energy infrastructure projects throughout the world.

13/01130 Estimation of the state-of-charge of gel lead-acid batteries and application to the control of a stand-alone wind-solar test-bed with hydrogen support

González, I. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11090–11103.

In hybrid renewable energy systems, batteries act as a DC bus to provide constant voltage and to smooth out commutations between the generating devices. These batteries are usually of a lead–acid type and operate under harsh variable conditions due to fluctuations of both solar radiation and wind speed. Precise knowledge of the state of charge (SOC) of the batteries, and hence of their available energy, play a key role in effecting efficient control and energy management of the installation. The present study had a twofold aim. One objective was to adjust and validate a method based on coulomb counting to estimate the SOC of a gelled lead–acid battery which is the DC bus of a hybrid wind–solar system with hydrogen storage. Other works evaluate SOC models based on several parameters, however, the present proposal based on experimental measurements involves only a few parameters. The second objective was to modify the installation's control algorithm to use the battery's calculated SOC as control parameter instead of its voltage. The results of a test-bed system, showing how the system evolved under real operating conditions, constitute a proof of concept of the validity of the method.

13/01131 Implications of biomass pretreatment to cost and carbon emissions: case study of rice straw and Pennisetum in Taiwan

Chiueh, P. T. *et al. Bioresource Technology*, 2012, 108, 285–294.

The purpose of this study was to explore the impact of feedstock collection and torrefaction pretreatment on the efficiency of a biomass co-firing system. Considering the transformation of existing municipal solid waste incinerators, several scenarios in which biomass supply chains depend on centralized pretreatment and transportation alternatives are presented. The cost, net energy output, and greenhouse gas effects of these scenarios were analysed using a spreadsheet model. Based on the Taoyuan County case in Taiwan, the mitigation costs of carbon emissions for rice straw and Pennisetum are \$77.0/Mg CO_2 and \$63.8/Mg CO_2, respectively. Results indicate that transporting feedstock from its source to the pretreatment and co-firing stations contributes the most to logistical costs for both straw and Pennisetum, regardless of whether torrefaction was adopted. Nonetheless, torrefaction requires more demonstrated cases at various scales to obtain the technical and economic data required for further analysis.

13/01132 Neural control for wave power plant during voltage dips

Amundarain, M. *et al. Electric Power Systems Research*, 2012, 92, 96–105.

The present paper proposes a strategy based on a novel neural control by means of a doubly fed induction generator to improve the performance of the wave energy converter during voltage dips in the grid. A neural control strategy is employed to coordinate the active crowbar, the air valve control and the back to back control. For this purpose, the neural controller adapts the references according to the voltage reduction and pressure drop improving the controllability of the active and reactive power and the fault-ride-through capability during voltage sags. Simulation results are included so as to demonstrate the viability of the proposed control.

13/01133 Optimal energy management of small electric energy systems including V2G facilities and renewable energy sources

Battistelli, C. *et al. Electric Power Systems Research*, 2012, 92, 50–59.

The emerging of plug-in hybrid vehicles results not only in the increase of electric vehicles as means of transportation, but also in the utilization of vehicle batteries for grid support, which is referred to as vehicle to grid (V2G). However, V2G is still at a conceptual stage, and the lack of practical and realistic frameworks to help moving from concept to implementation causes serious challenges to its adoption. In this context, this paper proposes a practical model for the assessment of the contribution of V2G systems as a support to energy management within realistic configurations of small electric energy systems (SEESs) including renewable sources, such as microgrids. Considering the uncertainty factors related to renewable power sources and gridable vehicles, the model materializes into a robust linear optimization problem suited to be easily integrated in the Energy Management System of SEESs, to support – in operation or operation planning – SEESs' participation in the electricity market. The paper also presents a practical methodology to model the aggregation of gridable vehicles, contributing to the literature in the field and helping towards the actual implementation of V2G. The efficiency and usefulness of the developed aggregation and optimization models are shown using a realistic SEES case study.

13/01134 Potential energy production from algae on marginal land in China

Zhang, Q. *et al. Bioresource Technology*, 2012, 109, 252–260.

This study is aimed to systematically estimate marginal land resources with different grades (total area; land with certain eco-environmental-economic feasibility; centralized reserve land) in China, and evaluate potential energy production from microalgae on marginal lands in the long-, mid- and near-term, based on a model. The annual potential energy production from algae in total marginal land of China (APEMC) was estimated to 4.19 billion standard coal equivalent (tce), far more than total annual energy consumption equivalent in China (TECCE) in 2007. For microalgae with 35% lipid content, the APEMC in the mid-term would be 37.6–65.8% of the TECCE in 2007. The corresponding annual CO_2 emission mitigation by replacement of fossil fuels by algal bioenergy would be 4.27–7.44 billion t. Although Southwest China provides the highest potential algae production in the long-term, Northwest China provides the highest value in the near-term.

13/01135 Renewable energy: role of cooperation in entrepreneurship development

Vaghefpour, H. and Zabeh, K. *Energy Procedia*, 2012, 18, 659–665.

This paper discuss role of cooperation in creating opportunities for using rich renewable energy sources and also their potential role for entrepreneurship and employment in Iran. The presence of constant, sustainable and economical energy is an essential basis for any economic and social development while it can upgrade life qualities. Iran has a considerable amount of natural resources for modernizing its energy supply and being transited to a sustainable energy system as it has countless opportunities for using rich renewable energy sources. On the other hand, cooperation have been considered as a strategic way to create job opportunities as they are strong organizations which can encounter economic and social side-effects caused by quick moderating procedures in structural programs. Results show convergence between renewable sources development and Iran's economic development through taking a frugal approach in expenses, creating new job opportunities and entrepreneurship in renewable energies.

13/01136 Seasonal sea wave energy at al-Manara station in Tartous

Ibrahim, B. *et al. Energy Procedia*, 2012, 19, 104–105.

This paper shows that the variations of the total and significant seasonal sea wave energy at al-Manara station in Tartous. The authors used the wind speed data from the general metrological administration located in Damascus for duration of 6 years from the beginning of 1998 until 2003. The measurements were taken every hour. After the calculation of the total seasonal sea wave energy it was noticed that the energy had the values between 811 and 1608 J/m^2 in al-Manara area, while the seasonal significant sea wave energy values ranged between 2424 and 3830 J/m^2. The maximum sea energy was found in winter season.

13/01137 Wave energy potential along the northern coasts of the Gulf of Oman, Iran

Saket, A. and Etemad-Shahidi, A. *Renewable Energy*, 2012, 40, (1), 90–97.

This study aims to investigate wave power along the northern coasts of the Gulf of Oman. To simulate wave parameters the third generation spectral SWAN model was utilized, and the results were validated with buoy and ADCP data. First, annual energy was calculated in the study region with the hindcast data set covering 23 years (1985–2007). The areas with the highest wave resource were determined and the area proximity to the port of Chabahar is suggested as the best site for the installation of a wave farm. Second, the average monthly wave energy in this area was investigated. The most energetic waves are provided by the southeast Indian Ocean monsoon from June to August. Finally, the wave energy resource was characterized in terms of sea state parameters. It was found that the bulk of annual wave energy occurs for significant wave heights between 1 and 3 m and energy periods between 4 and 8 s in the direction of SSE.

14 FUEL SCIENCE AND TECHNOLOGY

Fundamental science, analysis, instrumentation

13/01138 A new method for improving critical extrapolation

Shang, X. *et al. Progress in Nuclear Energy*, 2012, 59, 44–48.

The divergent phenomenon of critical extrapolation and ρ–1/N extrapolation curve is analysed during the physical startup of a reactor. Aiming at the deficiency of the existing improving method – constant neutron source elimination (CNSE) method, a new method – variable neutron source elimination (VNSE) is proposed. This new method aims at getting accurate neutron count rate for extrapolation, and considers all the errors caused by the neutron source leakage, reactor spatial effect and neutron detector positions as a whole. Applied to a small reactor, this VNSE method can remove all errors and eliminate the divergence of extrapolation so that the accurate ρ–1/N extrapolation curve is got. The VNSE method is efficient and accurate for the critical extrapolation.

13/01139 A petascale direct numerical simulation study of the modelling of flame wrinkling for large-eddy simulations in intense turbulence

Hawkes, E. R. *et al. Combustion and Flame*, 2012, 159, (8), 2690–2703.
A new set of petascale direct numerical simulations (DNS) modelling lean hydrogen combustion with detailed chemistry in a temporally evolving slot-jet configuration is presented as a database for the development and validation of models for premixed turbulent combustion. The jet Reynolds number is 10,000, requiring grid numbers up to nearly seven billion, which was achieved by computation on 120,000 processor cores. In contrast to many prior DNS studies, a mean shear exists that drives strong turbulent mixing within the flame structure. Three cases are simulated with different Damköhler numbers, while Reynolds number is held fixed. Basic statistics are presented showing that integrated burning rates up to approximately six times the laminar burning rate are obtained. It is shown that increased flame surface area accounts for most of the enhanced burning while increases in the burning rate per unit area also play an important contribution. The database is then used to assess a new model of flame wrinkling intended for large-eddy simulations. The approach draws on concepts from fractal geometry, requiring the modelling of an inner cut-off scale representing the smallest scale of flame wrinkling, and the fractal dimension controlling the resolution dependence of the unresolved flame surface area. In contrast to previous modelling, it is argued that the inner cut-off should be filter-size invariant in an inertial range. Then, dimensional and physical reasoning together with Damköhler's limiting scaling laws for the turbulent flame speed are used to infer the cut-off and fractal dimension in limiting regimes. Two methods of determining the fractal dimension are proposed: a static, algebraic expression or a dynamic approach exploiting a Germano-type identity. Finally the model is compared against the DNS in *a priori* tests and is found to give excellent results, quantitatively capturing the trends with time, space, filter size and Damköhler number.

13/01140 Accounting robustly for instantaneous chemical equilibriums in reactive transport: a numerical method and its application to liquid–liquid extraction modeling

Métivier, L. and Roussel, H. *Computers & Chemical Engineering*, 2012, 45, 50–61.
Reactive transport equations are used in numerous application fields: CO_2 or nuclear waste storage monitoring, separation processes in chemical engineering. The authors present a general method to account robustly for instantaneous chemical equilibriums in reactive transport. This method is adapted to all kinds of hydraulic transport models including 1D to 3D convection–diffusion equations. This leads to the resolution of a bound constrained system of differential algebraic equations (DAEs). The algebraic constraints come from the adjunction of mass action laws related to the equilibriums, whereas the bounds account for the positivity of the computed quantities. In order to solve the numerical system associated with this method, the authors use an adaptation of the DASSL solver, CDASSL, that can handle the resolution of bound constrained DAE systems. They present an application of this method to liquid–liquid extraction modelling. Numerical experiments demonstrate the interest of using the CDASSL solver to ensure the bound constraints are satisfied.

13/01141 An interactive multi-objective optimization framework for sustainable design of bioprocesses

Taras, S. and Woinaroschy, A. *Computers & Chemical Engineering*, 2012, 43, 10–22.
Interactive multi-objective optimization methods have considerable advantages over the other multi-objective optimization methods and are well suited for biochemical engineering problems. Interactive optimization is a very complex task which requires appropriate software to handle multiple objectives, displaying intermediary results and allowing the decision maker to specify preferences for each iteration. The proposed strategy combines Matlab and SuperPro Designer simulator. This way, the SuperPro Designer simulator benefits from the available toolboxes, computation, and visualization advanced features of Matlab. By linking Matlab and SuperPro Designer simulator, an optimization loop is created. This allows an automatically and repeatedly bidirectional exchange of variables between optimization algorithm from Matlab and SuperPro Designer simulator. In order to fully automate the optimization process, software based on component object module technology, which contains three friendly graphical interfaces, was created. The presented strategy is implemented for a L-lysine feed supplement plant, both economic and environmental objectives being considered.

13/01142 Analysis and design of the flexible composite membrane stretched on the spacecraft solar array frame

Morozov, E. V. and Lopatin, A. V. *Composite Structures*, 2012, 94, (10), 3106–3114.
Non-linear analysis of the deformation of a thin flexible composite membrane stretched on a rectangular cell of the spacecraft solar array frame is presented in the paper. The frame of the array and the thin flexible membrane stretched on this frame are designed to be capable of withstanding the transverse mechanical loadings exerted on the structure during the delivery to orbit and deployment. The governing non-linear equations modelling the pre-stretched flexible orthotropic membrane are solved using Galerkin method. Results of calculations are compared with those based on finite-element modelling. The comparisons have demonstrated efficiency of the proposed approach to the analysis and design of composite solar arrays featuring orthotropic composite flexible membranes. The parametric analyses were performed for various combinations of the g-force, mass of the photovoltaic elements and dimensions of the solar array.

13/01143 Application of the harmony search algorithm to calculate the interaction parameters in liquid–liquid phase equilibrium modeling

Merzougui, A. *et al. Fluid Phase Equilibria*, 2012, 324, 94–101.
The interaction parameter estimation problem in thermodynamic models is an important requirement and a common task in many areas of chemical engineering because these models form the basis for synthesis, design, optimization and control of process systems. Recently, this problem has been solved using minimization of Gibbs free energy, using global optimization techniques. In this paper, liquid–liquid equilibrium data of ternary system (water + alcohol + isopropyl ether) at 298.15 K is experimentally investigated, A newly developed heuristic algorithm, harmony search algorithm (HSA) is applied for solving the liquid–liquid phase equilibrium and estimation of binary interaction parameters of this ternary systems. The results of the proposed method are compared with the results given by other optimization techniques such as genetic algorithm. In all cases, the obtained solutions using the modified HSA are valuable.

13/01144 Approximate polynomial solutions for nonlinear heat transfer problems using the squared remainder minimization method

Căruntu, B. and Bota, C. *International Communications in Heat and Mass Transfer*, 2012, 39, (9), 1336–1341.
This paper introduces a new approximation method, called the squared remainder minimization method, which allows the analytical approximate polynomial solutions to be computed for several non-linear heat transfer problems. The applications illustrate the validity of the method and a comparison with previous results emphasizes the accuracy of the method.

13/01145 Artificial intelligence methods applied for quantitative analysis of natural radioactive sources

Medhat, M. E. *Annals of Nuclear Energy*, 2012, 45, 73–79.
Artificial neural network (ANN) represents one of artificial intelligence methods in the field of modelling and uncertainty in different applications. The objective of the proposed work was to apply ANN to identify isotopes and to predict uncertainties of their activities of some natural radioactive sources. The method was tested for analysing gamma-ray spectra emitted from natural radionuclides in soil samples detected by a high-resolution gamma-ray spectrometry based on high-purity germanium. The principle of the suggested method is described, including, relevant input parameters definition, input data scaling and networks training. It is clear that there is satisfactory agreement between obtained and predicted results using neural network.

13/01146 Biological monitoring for carbon capture and storage – a review and potential future developments

Noble, R. R. P. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 520–535.
Effective monitoring of carbon capture and storage (CCS) projects is essential, but detection of leaks and subsequent subtle changes in the surrounding environment are difficult to assess. New tools are being developed for this purpose, yet biological monitoring methods have been undervalued; this is surprising given the rapid technological expansion in the field of microbial ecology over the last decade. A review of biological monitoring for CCS shows a number of techniques such as plant surveys, bacterial counts and DNA fingerprinting that

have been applied to natural analogues or shallow injection sites. The results of the monitoring potential of these methods vary, perhaps explaining the limited research and adoption of biological monitoring for CCS projects. However, new tools such as microarrays provide rapid throughput that can characterize microbial populations and functional genes that may change due to CO_2 leakage and subsequent effects. These tools are not the whole answer for CCS monitoring, but they open new opportunities in this area and should lead to the development of simple biosensors and an expansion of the monitoring toolkit. Comparisons to other fields of research, such as tracing contaminants plumes of BTEX, demonstrate how the techniques reviewed can be developed and applied to CCS monitoring.

13/01147 Blast resistance and energy absorption of foam-core cylindrical sandwich shells under external blast

Fatt, M. S. H. and Surabhi, H. *Composite Structures*, 2012, 94, (11), 3174–3185.

The early time, through-thickness stress wave response of a foam-core, composite sandwich cylindrical shell under external blast is examined in this paper. Solutions for the transient response of the facesheets were derived as stress waves propagated through an elastic–plastic, crushable foam core. These solutions were found to be in good agreement with results from finite element analysis. The blast response of the composite sandwich cylindrical shell was shown to be affected by the magnitude and duration of the pressure pulse. High-amplitude, low duration (impulsive) pressure pulses induced the greatest energy absorption. Low amplitude, long duration pressure pulses caused minimal energy absorption. The amount of energy absorbed increased and the failure load decreased with increasing core thickness. Sandwich shells with foams of varying density, compressive modulus and crushing resistance were also examined. The sandwich shells with the foam of the highest density, compressive modulus and crushing resistance (Divinycell HCP100) were found to be the most blast resistant to failure even though no energy was absorbed by them. Per unit weight, however, the shells with a lighter, less stiff and strong, Divinycell H200 foam core were more blast resistant to failure than shells with a Divinycell HCP100 foam core.

13/01148 Comparison of optimal design methods for type 3 high-pressure storage tanks

Francescato, P. *et al. Composite Structures*, 2012, 94, (6), 2087–2096.

This study compares different optimal design methods for producing two-angle filament-wound structures able to withstand under internal pressure. In recent years, studies have concentrated on materials and their damage behaviour as well as winding optimization techniques in relation to vessel geometry and manufacturing processes, but none of these studies has established a definitive design rule. In the present paper, two developed methods, one based on a basic CPT with gradual damage and enumerative optimization, the other a more sophisticated finite element (FE) method with Reddy's progressive damage law and genetic algorithm (GA) optimization are compared to recent results based on CDM theory and a three-dimensional FE technique incorporating a modified GA. The results were used to compare the advantages and limitations of each method and to derive simple design rules and calculation strategies that would reliably obtain a very good computing cost/efficiency ratio.

13/01149 Competitive diffusion of gases in a zeolite using proton NMR and a slice selection procedure

Leclerc, S. *et al. Catalysis Today*, 2012, 187, (1), 104–107.

The study of the co-diffusion of several gases through a microporous solid and the resulting instantaneous distribution (out of equilibrium) of the adsorbed phases is particularly important in many fields, such as gas separation and heterogeneous catalysis. Classical ^1H NMR imaging is a good technique for the visualization of these processes but, since the signal obtained is not specific for each gas, this requires that each experiment be performed several times under identical conditions, and each time with only one incompletely deuterated gas. In contrast the authors have proposed a new NMR imaging technique (based on the so-called NMR lift) which gives a signal characteristic of each adsorbed gas. It can therefore provide directly, at every moment and at every level of the crystallite bed, the distribution of several gases competing in diffusion and adsorption.

13/01150 Computing the correlation between catalyst composition and its performance in the catalysed process

Holeňa, M. *et al. Computers & Chemical Engineering*, 2012, 43, 55–67.

The methodology for computing correlations between continuous descriptors of catalytic materials and their performance in the catalysed process is addressed. Continuous descriptors are typically molar fractions of individual components of the catalyst, whereas the performance is represented most frequently by yield or selectivity of reaction products or conversion of key feed components. Measures of various kinds of correlation are recalled, and their descriptor-wise application to catalytic data for computing correlations between the composition and performance of catalysts is presented. The paper also compares the application of correlation measures to catalytic data on the one hand with the analysis of variance, on the other hand with the application of regression trees. As a case study, the presented approaches are applied to data from high-temperature synthesis of hydrocyanic acid.

13/01151 Convex envelope method for the determination of fluid phase diagrams

Ryll, O. *et al. Fluid Phase Equilibria*, 2012, 324, 108–116.

In this work a new method – the convex envelope method (CEM) – for the reliable determination of fluid phase diagrams is presented. The method yields the entire phase equilibrium diagram and does not rely on the determination of individual equilibria. Formally, the CEM is based on the original idea of Gibbs interpreting all globally stable equilibrium states as those belonging to the convex envelope of the Gibbs energy over the composition space. In this work, the continuous Gibbs energy surface is approximated by an appropriate set of points. This allows a mathematically clear reformulation of the original problem as convex hull determination for a discrete set of Gibbs energy points and thus the continuous Gibbs energy surface itself. The CEM is quite generally formulated for any system with arbitrary coexisting (fluid and solid) phases. In this work it is applied to systems with multiple liquid phases only, since liquid multi-phase equilibrium diagrams are extremely important in practice for extraction and decanter design. The implementation of CEM relies on a numerical construction of the convex hull which determines the accuracy of the results. The CEM can be easily integrated in short-cut methods for analysis of separation methods based on liquid phase splitting. Therefore, the CEM is explained for the application to liquid multi-phase equilibria and validated with available experimental data and rigorous decanter simulations for several systems with complex phase behaviour.

13/01152 Crosswind action on rail vehicles: a methodology for the estimation of the characteristic wind curves

Cheli, F. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2012, 104–106, 248–255.

The problem of cross wind for rail vehicles gained, in the last years, an increasing interest within the European railway operators, due to the continuous expansion of the high-speed railway networks. In order to evaluate the aerodynamic performance of a train in terms of safety towards cross wind, the characteristic wind curves (CWCs), have to be defined. In this paper a stochastic approach for the definition of the CWCs is presented. According to this methodology, the wind speed space–time distribution is reproduced through a stochastic process and the algorithm for the definition of the aerodynamic loads acting on the train is set up, which is based on the admittance function. A numerical model for the admittance function is presented and verified by means of comparison with experimental data. The effects of the admittance function and of the stochastic approach in the definition of aerodynamic forces and of the corresponding CWCs are then analysed in terms for a specific case (assigned reference train, flat ground scenario, tangent track running).

13/01153 Effect of an axial electric field on detonation waves

Kamenskihs, V. and Lee, J. H. S. *Combustion and Flame*, 2012, 159, (9), 2967–2973.

This paper reports the results of an investigation of the effects of an axial electric field (200–8000 V/cm) on the propagation of detonation waves in mixtures of $2CO + O_2$ and $C_2H_2 + O_2 + 85\%Ar$. High-speed streak camera and photodiodes were used for detonation velocity measurements. In addition, the voltage across the axial electrodes and the current are monitored as the detonation traverses the electric field region. The present results show that the neither the detonation structure nor its velocity are influenced by the electric field as it traverses the region between electrodes except when a breakdown occurs ahead of the detonation. The breakdown is due to the progressively increasing electric field between the detonation (which acts like a travelling quasi-neutral conducting plasma slug) and the downstream electrode. For a sufficiently strong electric field an arc discharge develops between the detonation and the charged electrode. When a discharge occurs in the unburned mixture ahead of the detonation wave, the mixture is ignited prior to the detonation arrival. This leads to the failure of the detonation since it now propagates into burnt products. Re-initiation of the failed detonation may occur downstream of the discharge section.

13/01154 Energy storage devices to support functional movements' restoration

Massoud, R. *Energy Procedia*, 2012, 19, 63–70.

In this paper, the ways of employing energy storage devices in hybrid powered orthoses have been discussed. Since these devices have many unrivalled advantages, they are environmentally safe, they store kinetic energy as potential energy and release it when it is needed and they do not need external power supply. In this paper an energy storage device (linear extension spring) has been implemented in FES-cycling, the efficiency has been calculated for different spring positions and different spring constants. It was clear that FES-cycling efficiency increases when the spring constant increases, then the pedal, spring and the overall powers were calculated, and it appears that by leaning the spring position the overall power will be always positive, and the spring absorbs the exceeded pedal energy and releases it when the pedal power is negative. This study highlights the importance of using energy storage devices to improve FES-cycling performance, which has been proven that such improvement is highly related to the mechanical design of the bicycle.

13/01155 Enhanced thermal conductivity and specific heat capacity of carbon nanotubes ionanofluids

de Castro, C. A. N. *et al. International Journal of Thermal Sciences*, 2012, 62, 34–39.

Ionanofluids represent a new and innovative class of heat transfer fluids which possess fascinating thermophysical properties. They are designable and fine-tunable through their base ionic liquids. Experimental results on effective thermal conductivity and specific heat capacity of ionanofluids as a function of temperature and concentration of multi-wall carbon nanotubes in several ionic liquids are presented. Results showed that ionanofluids exhibit superior thermal conductivity and specific heat capacity compared to those of their base ionic liquids and they further increase with the concentration of carbon nanotubes. Although the enhancement of the effective thermal conductivity of ionanofluids was found to be independent of temperature, the specific heat capacity increases significantly with increasing temperature in the range of 60–90 °C. Interaction between ionic liquid ions and dispersed nanotubes is believed to be one of the key factors for the enhanced thermal conductivity of ionanofluids.

13/01156 Estimation of nuclear volume dependent fractionation of mercury isotopes in equilibrium liquid–vapor evaporation experiments

Ghosh, S. *et al. Chemical Geology*, 2012, 336, 5–12.

To confirm theoretical predictions of the isotopic signature of the nuclear volume effect (NVE) for Hg, liquid–vapour Hg isotope fractionation was investigated under equilibrium conditions in the dark at room temperature. Since the other mass independent fractionation (MIF) mechanism proposed for Hg is a kinetic phenomenon only, equilibrium experiments are the best approach to isolate the NVE. Because of the small magnitude of NVE MIF, previous equilibrium experimental results have had relatively large error. The equilibrium evaporation experiment resulted both in mass dependent fractionation (represented by δ^{202}Hg) and MIF (Δ^{199}Hg and Δ^{201}Hg). The average liquid–vapour δ^{202}Hg difference was $1.34 \pm 0.18‰$ (2SE) and $1.08 \pm 0.07‰$ (2SE) for two sets of experiments with the vapour phase isotopically lighter than the liquid. A positive MIF of the odd isotopes in the vapour phase was observed with an average Δ^{199}Hg of $0.14 \pm 0.01‰$ (2SE) and an average Δ^{201}Hg of $0.09 \pm 0.01‰$ (2SE). For the six experiments, the average ratio of NVE MIF of the two odd isotopes (Δ^{199}Hg/Δ^{201}Hg) in the vapour phase was 1.59 ± 0.05 (2SE) confirming a recent estimation of the NVE Δ^{199}Hg/Δ^{201}Hg ratio of ~1.65. A conceptual model applying first principles was used to explain the fractionation observed between Hg liquid and Hg vapour under equilibrium conditions.

13/01157 Experimental investigation on the seepage law of pressure-relieved gas under the influence of mining

Li, S. *et al. Safety Science*, 2012, 50, (4), 614–617.

The stress distribution characteristics of the coal seam floor and the variation of pressure-relieved gas seepage velocity along with working face being advanced were studied experimentally. According to experimental data, the distribution rule and the influence area of abutment pressure of gob floor were analysed. The scope of 'three zones' formed by gas seepage velocity along lateral direction above the gob was determined, and the coupling rule of pressure-relieved gas was summarized. The above results provide a technical support for the spot gas extraction.

13/01158 Experimental study of distribution of energy during EDM process for utilization in thermal models

Singh, H. *International Journal of Heat and Mass Transfer*, 2012, 55, (19–20), 5053–5064.

Electrical discharge machining (EDM) has steadily gained importance over the years because of its ability to cut and shape a wide variety of materials and complicated shapes with high accuracy. The effectiveness of the EDM process is evaluated in terms of the material removal rate, relative wear ratio and the surface roughness of the work piece. The input discharge energy during this process is distributed to various components of the process, which further influences the material removal rate and other machining characteristics like surface roughness. Since during this process the electrical energy is converted into heat energy, hence the theoretical modelling of this process is based upon the heat transfer equations and in all existing thermal models the fraction of the energy transferred to the workpiece, is one of the important parameters. The accurate prediction of the fraction of energy effectively transferred to the workpiece will help to reduce the errors of the thermal models. In this study experiments have been performed to study the percentage fraction of energy transferred to the workpiece utilizing heat transfer equations, at different EDM parameters. This study also relates the optimum parameters with the optimum utilization of input discharge energy and hence will help to improve the technological performance of this process.

13/01159 Experimental study of water wetting in oil–water two phase flow – Horizontal flow of model oil

Cai, J. *et al. Chemical Engineering Science*, 2012, 73, 334–344.

When crude oil and water are simultaneously transported in mild steel pipelines, corrosion problems are generally associated with the water phase being in contact with the metal surface at the bottom of the pipe. Consequently, knowing whether oil or water wets the pipe wall is an important factor, which can affect the corrosion mitigation strategy and increase confidence in the integrity of the pipeline. There are large knowledge gaps in this area of research and consequently only very crude empirical criteria are used in the industry. In the present work an experimental study of oil–water flow was conducted in a large diameter (0.1 m ID) horizontal multiphase flow loop using four measurement techniques: flow pattern visualization, conductivity pins, fluid sampling and monitoring of corrosion rate via ferrous ion concentration (iron count). Five different oil/water flow patterns were observed and a flow regime map was constructed. The flow patterns were smooth stratified flow, stratified flow with water globules, stratified flow with mixing layer, semi-dispersed flow and dispersed flow. The results from the conductivity pins showed three different wetting behaviours: stable water wetting, stable oil wetting and intermittent wetting. The results of the fluid sampling were consistent with the wetting results from the conductivity pins. Ferrous ion monitoring demonstrated that corrosion occurs only when water wets the pipe walls and is greater for stable water wetting than for intermittent wetting.

13/01160 First principles calculation of noble gas atoms properties in 3C–SiC

Eddin, A. C. and Pizzagalli, L. *Journal of Nuclear Materials*, 2012, 429, (1–3), 329–334.

First-principles calculations were performed to investigate the properties of single noble gas (NG) atoms (He, Ne, Ar, Kr, Xe) in 3C–SiC. The stability of a NG atom was investigated in the presence or not of a mono-vacancy (or di-vacancy). In a perfect lattice, the most stable interstitial configuration were T^{Si} (He and Ne), and BC (Ar, Kr and Xe). It was found that mono-vacancy V^{Si} and V^{C} are traps for a single NG atom, with a lower formation energy for NG-V^{Si}. Heavier NG species prefer to occupy the vacancy, whereas He is more stable in its vicinity. NG species tend to remain in di-vacancies, with low formation energies. A simple analysis demonstrates that at equilibrium, Ar, Kr and Xe interstitials are unlikely to exist since it is energetically cheaper to create a mono-vacancy or di-vacancy. This would suggest that the ejection of self-interstitials should play a major role in the formation and evolution of bubbles filled with heavy NG species. This is in agreement with the experimental observations of a larger density of dislocation loops in the case of Xe compared to Ne. Finally, the authors investigated the migration of He, Ne and Ar interstitials through successive hoppings between T^{Si} and T^{C} sites. The migration energy barriers are determined to be 1.49, 1.92 and 1.81 eV, respectively. Using the computed migration and formation energies for He, it can be shown that the energy required for the dissociation of He–V or He–V_2 complexes and the subsequent desorption ranges between 3.1 and 3.3 eV, in good agreement with experiments. Note that this could be accidental since the influence of temperature and pressure, which should be taken into account, were not considered here. The calculations also hinted that the growth of He-filled bubbles is likely to happen through the migration of He interstitials. Nevertheless, it will be necessary to investigate the migration of NG-mono or di-vacancy complexes, for He but also for larger NG atoms, to draw more definitive conclusions.

13/01161 Hydrozincite seasonal precipitation at Naracauli (Sardinia – Italy): hydrochemical factors and morphological features of the biomineralization process

Medas, D. *et al. Applied Geochemistry*, 2012, 27, (9), 1814–1820.

Hydrozincite [$Zn_5(CO_3)_2(OH)_6$] precipitation from Naracauli waters (south-west Sardinia) is, among other things, promoted by a microbial community made up of a filamentous cyanobacterium (*Scytonema* sp.) and a microalgae (*Chlorella* sp.). Hydrozincite bioprecipitation is responsible for the natural removal of harmful metals, especially Zn, from the stream waters. Thus, hydrozincite could be used to attenuate metal pollution in mining waters. Information on environmental conditions which promote the biomineralization process is fundamental for the development of remediation strategies. This paper aims to investigate the variables controlling the biomineralization process, and seasonal variation of the hydrochemical factors that affect hydrozincite precipitation. Hydrozincite morphology varies depending on the environmental conditions. Specifically, changes were observed between samples collected in late spring and samples collected in summer, and among samples precipitated under different water flow conditions. According to field observations, correlated with speciation and equilibrium calculation, the maximum intensity in hydrozincite precipitation occurs in the late spring during rainy years. In these conditions, the hydraulic regime in the stream reaches stationary conditions, and saturation index values with respect to hydrozincite reach their highest values. Concomitantly, the Zn^{2+}/CO_3^{2-} molar ratio reaches values close to 1, indicating that kinetic processes have a role on the hydrozincite biomineralization process.

13/01162 Measurement of electrical properties of refrigerants and refrigerant–oil mixtures

Feja, S. *International Journal of Refrigeration*, 2012, 35, (5), 1367–1371.

The paper deals with the description of a new pressure proof device developed at ILK Dresden for measuring electrical properties of refrigerants, oils and refrigerant–oil mixtures under pressure. The determination can be performed based on DIN EN 60247. This standard is valid for the determination of the relative permittivity, the dielectric dissipation factor and the direct current resistivity of isolating fluids at atmospheric pressure. The measurements can be made in a temperature range from −30 to 90 °C at pressures up to 80 bar under dry atmospheric conditions. The sensitivity of the method as well as its considerable flexibility meets the requirements of the industrial and commercial refrigeration. Challenges regarding the development and performance of the measuring cell as well as some preliminary experimental results are presented. The focus of the experiments is on environmentally friendly refrigerants ($GWP < 150$) such as R744, R1234yf and R152a, and their mixtures with lubricants.

13/01163 Modeling typhoon wind power spectra near sea surface based on measurements in the South China sea

Li, L. *et al. Journal of Wind Engineering and Industrial Aerodynamics*, 2012, 104–106, 565–576.

This study focuses on enhancing the understanding of the spectral features of typhoon winds with critical implications on the mitigation of disproportionate damage experienced in typhoon-prone coastal regions. Examination of data suggests that generally used empirical models of wind power spectrum for extratropical storms may not adequately represent the tropical cyclone winds. In this paper, a data-driven model is proposed for wind power spectrum in tropical cyclone winds over the sea surface. Rather than fitting data to a universal spectral description, first the physical meaning of parameters in such a model is carefully examined and the contribution of each parameter is delineated. With these backgrounds, field measurements in typhoon Hagupit are used to model these spectral parameters in terms of the Monin–Obukhov length, mean wind speed and roughness length. Finally, the proposed spectral model is validated using arbitrarily selected four hours of data in different sectors of typhoon Hagupit wind field. The model shows a good agreement with the measurements.

13/01164 Multiscale analysis of geomorphological and geological features in high resolution digital elevation models using the wavelet transform

Kalbermatten, M. *et al. Geomorphology*, 2012, 138, (1), 352–363.

At the end of the 1990s the emergence of high resolution (1 m) digital elevation models (DEMs) settled the context of high precision geomorphological analysis. These new elevation models permitted to reveal structures that remained heretofore undetectable. Earth scientists henceforth benefit from a source of data with a textural detail that was never attained before. Despite its richness, this information must be treated efficiently to extract features helping geomorphologists to analyse the processes occurring at the surface. Such processes are complex, localized and naturally multiscale. Recently, space-frequential descriptors as wavelets have been proposed successfully for the analysis of DEMs. The wavelet transform is widely used in image processing since it allows us to decompose a signal into a weighted sum of atoms with joint space-frequency localization. Such a decomposition facilitates a coherent navigation from scale to scale, but also permits to detect heretofore undiscerned phenomena at different scales. This is appealing in geomorphology, where structural components, related to a given phenomenon, are well determined in these sub-spaces specific to the scale continuum. In this paper, the authors propose a filtering procedure of the wavelet decomposition as an approach for the analysis of geomorphological multiscale structures. This filtering procedure enhances the high pass information contained at each scale. The proposed bottom–up approach is applied here to a case study to detect geomorphological structural elements in a valley of the Swiss Jura. It demonstrates that the proposed filtering procedure is an efficient tool for geomorphological multiscale generalization.

13/01165 Neutronics diagnostics for European ITER TBMs: activation foil spectrometer for short measurement cycles

Klix, A. *et al. Fusion Engineering and Design*, 2012, 87, (7–8), 1301–1306.

An important aim of neutronics test blanket module (TBM) experiments in ITER will be to check the prediction accuracy of nuclear responses in an environment closer to a future fusion power reactor than so far provided by existing facilities. The development of measurement methods suitable for the harsh environment in an ITER TBM has been addressed in several recent R&D programs supported by Euratom. Within this framework, KIT is developing an activation foil spectrometer for the measurement of local neutron flux densities in the TBM. The authors intend to establish a measurement method which allows to record the induced activities in small packages of activation foils simultaneously and to calculate the corresponding spectral neutron flux densities with moderate time resolution of tens of seconds immediately after extraction from the TBM. This paper proposes a candidate set of activation foil materials which cover the neutron energy range from thermal to 1 MeV. In order to assess their basic suitability for such measurements, the authors have computed induced gamma-ray activities in the foils using a calculated neutron spectrum in a representative position in the European HCPB TBM assuming a short irradiation time of 30 s. In a further step the authors have investigated pulse height spectra which would be obtained in a typical gamma-ray measurement arrangement in a HPGe detector and concluded that the proposed set of activation foils should be basically suitable for such a measurement system but require improvement of relevant cross sections uncertainties.

13/01166 Numerical sensitivity study of thermal response tests

Wagner, V. *et al. Renewable Energy*, 2012, 41, 245–253.

Thermal conductivity and thermal borehole resistance are basic parameters for the technical and sustainable design of closed ground source heat pump (GSHP) systems. One of the most common methods to determine these parameters is the thermal response test (TRT). The response data measured are typically evaluated by the Kelvin line source equation which does not consider all relevant processes of heat transfer in the subsurface. The approach only considers conductive heat transfer from the borehole heat exchanger (BHE) and all transport effects are combined in the parameters of effective thermal conductivity and thermal borehole resistance. In order to examine primary effects in more detail, a sensitivity study based on numerically generated TRT data sets is performed considering the effects of (1) the *in situ* position of the U-shaped pipes of borehole heat exchangers (shank spacing), (2) a non-uniform initial thermal distribution (such as a geothermal gradient) and (3) thermal dispersivity. It will be demonstrated that the shank spacing and the non-uniform initial thermal distribution have minor effects (less than 10%) on the effective thermal conductivity and the determined borehole resistance. Constant groundwater velocity with varying thermal dispersivity values, however, has a significant influence on the thermal borehole resistance. These effects are even more pronounced for interpreted effective thermal conductivity which is overestimated by a factor of 1.2–2.9 compared to the real thermal conductivity of the saturated porous media.

13/01167 On chaotic advection in a static mixer

Saatdjian, E. *et al. Chemical Engineering Journal*, 2012, 187, 289–298.

The authors present a numerical study of chaotic advection and mixing in a spatially periodic, three-dimensional flow. The flow inside a cylindrical tube, into which one or more Kenics KM static mixer elements are inserted to promote mixing, is studied by solving the momentum equations numerically and then applying tools for analysis of mixing in time-periodic two-dimensional and three-dimensional chaotic flows. It is found that for this particular static mixer geometry, the initial location of a blob of dye is important for its spreading over the cross section of the tube only in the first few mixing elements, its influence decreases afterwards. The influence of the Reynolds number on mixing is mainly a finer grain of the resulting mixture, this is visible after several elements. A symmetry breaking modification of the standard Kenics KM static mixer geometry is suggested and subject to the same analysis as the original geometry. A slight improvement in the mixing efficiency is obtained with the modified geometry: it increases the extensional efficiency and gives a more homogeneous distribution of the stretching rates.

13/01168 On different types of adjustment usable to calculate the parameters of the stream power law

Demoulin, A. *et al. Geomorphology*, 2012, 138, (1), 203–208.

Model parameterization through adjustment to field data is a crucial step in the modelling and the understanding of the drainage network response to tectonic or climatic perturbations. Using as a test case a data set of 18 knickpoints that materialize the migration of a 0.7-Ma-old erosion wave in the Ourthe catchment of northern Ardennes (western Europe), the authors explore the impact of various data fitting on the calibration of the stream power model of river incision, from which a simple knickpoint celerity equation is derived. The results show that statistical least squares adjustments (or misfit functions) based either on the stream-wise distances between observed and modelled knickpoint positions at time t or on differences between observed and modelled time at the actual knickpoint locations yield significantly different values for the *m* and *K* parameters of the model. As there is no physical reason to prefer one of these approaches, an intermediate least-rectangles adjustment might at first glance appear as the best compromise. However, the statistics of the analysis of 200 sets of synthetic knickpoints generated in the Ourthe catchment indicate that the time-based adjustment is the most capable of getting close to the true parameter values. Moreover, this fitting method leads in all cases to an *m*-value lower than that obtained from the classical distance adjustment (for example, 0.75 against 0.86 for the real case of the Ourthe catchment), corresponding to an increase in the non-linear character of the dependence of knickpoint celerity on discharge.

13/01169 Optimum design of limaçon gas expanders based on thermodynamic performance

Sultan, I. A. *Applied Thermal Engineering*, 2012, 39, 188–197.

Positive displacement expanders have acquiring popularity due to the current push to harvest energy from low-grade heat resources which have been previously overlooked. The limaçon technology does offer a simple and reliable design with a considerable potential for small-size ($\leq$4 kW) power plants. A thermodynamic model was written and solved numerically at incremental values for the crank shaft angular motion. The model was then utilized in an optimization procedure to obtain the geometric parameters that would maximize the expander performance for specific power and operating constraints. Two numerical examples have been presented to highlight the fact that the expander performance can be greatly improved if a control valve has been fitted to the inlet port. The results of the numerical examples prove the validity of the models presented and their suitability for expander design.

13/01170 Pebble bed micro model system identification

Venter, W. C. and Lamprecht, E. C. *Annals of Nuclear Energy*, 2012, 46, 1–10.

Linear system identification techniques will be applied to obtain mathematical models of a simulation of the pebble bed micro-model (PBMM). The PBMM is a conceptual model of the pebble bed modular reactor (PBMR), a new high temperature gas nuclear reactor. Mathematical models for the transfer functions of nitrogen injection, nitrogen extraction and compressor bypass valve opening in the PBMM system have been obtained in this paper. These mathematical models are necessary for the development of an effective control strategy for the PBMM and PBMR plants. If necessary, the models can be reduced to second order if required, but the third-order models are more exact in describing the system behaviour. In the next phase of the project, system identification will be applied to obtain the transfer functions of the implemented PBMM plant. Attention will also be given to the development of multi-input single-output transfer functions for the plant when a combination of the possible inputs is applied at once.

13/01171 Precipitation enthalpy during cooling of aluminum alloys obtained from calorimetric reheating experiments

Zohrabyan, D. *et al. Thermochimica Acta*, 2012, 529, 51–58.

Precipitation reactions inside aluminium alloys are known to be very important for hardness and yield strength. Premature precipitation during quenching from solution annealing decreases the yield strength after aging. A methodology to determine the amount of precipitates as a function of quench rate (quench sensitivity) for a wide range of aluminium alloys from calorimetric reheating scans is proposed. The method allows determining the critical cooling rate for suppressing precipitation during quenching. Differential fast-scanning calorimetry was applied to cover the cooling rate range needed for high alloyed materials. The critical cooling rate for the quench sensitive EN AW 7049A alloy was determined as 300 K/s. A new methodology, called differential reheating method, was applied for differential fast-scanning calorimetry (DFSC) and differential scanning calorimetry (DSC). The method was quantitatively verified with EN AW 6063 alloy in a DSC due to its low critical cooling rate. The combination of DSC and DFSC extends the available cooling rate range for precipitation studies from mK/s up to some 10,000 K/s.

13/01172 Prediction of strain in a shaft caused by underground mining

Kwinta, A. *International Journal of Rock Mechanics and Mining Sciences*, 2012, 55, 28–32.

Displacements and strains due to mining can lead to damage to objects on the terrain surface and in the rock mass. Due to their importance, the functionality of main shafts of a mine must be secure. In order to make these shafts secure mining within their surroundings is limited or carried out by special methods. Continuous displacements due to a mining activity are forecast by means of the Knothe method with amendments. This method is used in case of both objects on the ground surface, and mine shafts. Commonly horizontal and vertical strains are determined separately. In order to assess threats to shafts due to continuous displacements, one should determine main spatial displacement along the entire shaft tube. This work presents a method to determine the main spatial deformations. Results and discussion are illustrated on an example.

13/01173 Primary study of temperature distribution measurement in stored grain based on acoustic tomography

Yan, H. *et al. Experimental Thermal and Fluid Science*, 2012, 42, 55–63.

A common and traditional method for detecting stored grain deterioration is the measurement of grain temperature. This study proposes a temperature monitoring method for stored grain based on acoustic tomography. A model describing the relationship between grain temperature and sound travel time in stored grain is established. A speed conversion coefficient is defined and used to convert the measured velocity of sound in the stored grain into the sound velocity in free space, which has the same gas components and temperature as those of the stored grain. The influence factors of the speed conversion coefficient are analysed, and the calibration method of the coefficient is introduced. The time-delay estimation method based on triple correlation and wavelet de-noising and the temperature reconstruction algorithm based on Markov radial basis function and singular value decomposition are used to measure the temperature distribution of the grain bulk. Two experimental systems are built to verify the acoustic model and reconstruct the temperature distribution of grain. The experimental result shows that the acoustic model can be used for temperature measurement in soybeans. The temperature distributions with different hot spot locations in soybeans are all well reconstructed, and the coordinates of the hot spots are reconstructed with better accuracy than that in thermocouple measurement. Thus, acoustic temperature measurement is useful in the early prediction of temperature anomalies in stored grain.

13/01174 Quantitative temperature profiling through null-point scanning thermal microscopy

Chung, J. *et al. International Journal of Thermal Sciences*, 2012, 62, 109–113.

This study develops and demonstrates the theory and method of null-point scanning thermal microscopy, which can obtain quantitative temperature profiles even when the heat conductance between the tip and the sample is disturbed due to abrupt changes in the surface topography or properties. Due to its generality, it would be widely applicable for a variety of problems associated with the thermal characterization of nanomaterials and nanodevices.

13/01175 Quench protection tests of a cryocooler cooled 6 T NbTi superconducting magnet by an active power method

Nanato, N. *et al. Cryogenics*, 2012, 52, (7–9), 321–324.

When a quench occurs in a superconducting magnet, excessive joule heating may damage the magnet. The authors have presented the quench protection system based on an active power method. The previous quench protection tests have been carried out for small superconducting magnets whose self-inductances are less than several hundred mH to verify the principles of the proposed system. This paper presents experimental results of quench protection tests of a cryocooler-cooled 6 T NbTi superconducting magnet (self-inductance 15.5 H), which is a commercial size magnet made by Tamakawa Co., Ltd. The authors confirmed that their proposed system could inhibit the maximum temperature of the superconducting magnet (initial temperature 4.3 K) after the quench to less than about 44 K at operation magnetic field 5.5 T. Experimental results suggest that the proposed system is useful for practical used superconducting magnets.

13/01176 Rockburst hazard determination by using computed tomography technology in deep workface

Dou, L. *et al. Safety Science*, 2012, 50, (4), 736–740.

The rockburst in mines results from the dynamic load coupled with static one in coal seams around workface zones, so it is essential to learn the stress distribution of the coal and surrounding rock for determination of rockburst risk areas. The relationship between the elastic wave velocity and stress applied on coal sample was investigated systematically by laboratory testing, theoretically analysis, as well as on-site observation, and a positive correlation between them under uniaxial compression was put forward. Furthermore, it is drawn that the anomaly of elastic wave velocity reflects the stress changes: the positive anomaly ascertains the stress concentration while the negative anomaly estimates the mining destress and weaken degree, and corresponding assessment criterions and parameters were established respectively. The hazard areas and degree of an island longwall face 16302C were forecasted before coal winning based on the elastic wave anomaly distribution rules using active tremor velocity inversion, monitoring results of mining shocks during exploitation indicate that the consistency between locations of big tremors and where forecasted by computed tomography exceed 80%. The successful application of this technology achieved remarkable economic and social benefits for disaster control in rockburst mines.

13/01177 Scaling up experiments of honeycomb catalysts for oxidation of hydrogen and methane gases

Uda, T. *et al. Fusion Engineering and Design*, 2012, 87, (5–6), 900–904.

For a large volume air cleanup system in nuclear fusion facility honeycomb type oxidizing catalyst offers more useful advantage in terms of their low pressure drop than the conventional particle packed bed. Scaling up examination of 35 times large volume Pd catalyst deposit on metal honeycomb Al–Cr-steel alloy had been performed comparing with fundamental small size honeycomb. The catalyst was heated up to over 400 °C with stepwise by combined the inner and external heaters under various flow rate of processing gas containing various concentrations of hydrogen and methane. Then oxidizing reaction rates and the catalytic activation energies were evaluated and thermal property of catalyst bed was estimated considering exothermic oxidizing reaction in the process gas. As a result it was revealed that the scaling up honeycomb catalyst bed would be practically useful for the air cleanup system.

13/01178 Solving dynamic economic dispatch problem with security constraints using bacterial foraging PSO-DE algorithm

Vaisakh, K. *et al. International Journal of Electrical Power & Energy Systems*, 2012, 39, (1), 56–67.

This paper presents a heuristic optimization methodology, namely, bacterial foraging PSO-DE (BPSO-DE) algorithm by integrating bacterial foraging optimization algorithm (BFOA), particle swarm optimization (PSO) and differential evolution (DE) for solving non-smooth non-convex dynamic economic dispatch (DED) problem. The DED problem exhibits non-smooth, non-convex nature due to valve-point loading effects, ramp rate limits, spinning reserve capacity, prohibited operating zones and security constraints. The proposed hybrid method eliminates the problem of stagnation of solution with the incorporated PSO and DE operators in original bacterial foraging algorithm. It achieves global cost by selecting the bacterium with good foraging strategies. The bacteria with good foraging strategies are obtained in the updating process of every chemo-tactic step by the PSO operator. The DE operator fine tunes the solution obtained through bacterial foraging and PSO operator. A three- and seven-unit systems for static economic dispatch, a 26-bus, six-generator test system and an IEEE 39-bus, 10-unit New England test systems are considered to show the effectiveness of the proposed method over other methods reported in the literature.

13/01179 Stability analysis of non-isothermal film blowing process for non-Newtonian fluids using variational principles

Kolarik, R. *et al. Chemical Engineering Science*, 2012, 73, 439–453.

In this study, a numerical stability analysis of the film blowing process is performed. The numerical scheme used is based on a variational principle model of the film blowing operation. This model employs non-isothermal processing conditions, non-Newtonian behaviour of the polymer and physically limiting criteria (maximum tensile and/or hoop stress) to investigate the complex relationship between processing conditions (internal bubble pressure, heat transfer coefficient, mass flow rate, cooling air temperature, melt/die temperature), material parameters (rupture stress, Newtonian viscosity, flow activation energy, power law index) and film blowing stability. It has been shown that the melt/die temperature has the highest impact on the film blowing stability window size as well as on the maximum and minimum achievable film thickness. In more detail, it has been found that processing parameters together with flow activation energy have much higher effect on the film blowing stability and maximum achievable film thickness than the basic rheological characteristics of the polymer melt. On the other hand, the effect of basic rheological parameters of the polymer melt become much more important than processing parameters (except of melt/die temperature) in order to reach minimum film thickness.

13/01180 Study on steam-carrying effect in static flash evaporation

Zhang, D. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (17–18), 4487–4497.

Study on steam-carrying effect in static flash of both pure water and aqueous NaCl solution was present. Properties, including steam-carrying ratio, waterfilm height drop and equilibrium concentration of waterfilm, were measured in experiments. Their dependences on separating height, initial waterfilm concentration and mean pressure difference were analysed. Particularly, steam-carrying ratio was defined as the mass ratio of be-carried liquid and generated steam. Results suggested that this ratio increased with the decreasing of separating height or the rising of initial waterfilm concentration, and a peak value existed in its evolution versus mean pressure difference. At last, according to experimental results and basic principles a calculating model for steam-carrying effect in static flash was built.

13/01181 The effect of nonhomogeneity and end supports on the thermo elastic behavior of a clamped–clamped FG cylinder under mechanical and thermal loads

Arefi, M. and Rahimi, G. H. *International Journal of Pressure Vessels and Piping*, 2012, 96–97, 30–37.

This paper deals with the thermoelastic analysis of a clamped–clamped functionally graded cylinder under internal pressure. Hamilton principle and first-order shear deformation theory (FSDT) are employed for derivation of the principle differential equations. Solution of these differential equations includes the particular and homogenous solutions. Homogenous solution can be obtained by recognizing the imaginary and real roots of characteristic equation. With imposing the natural boundary condition at the end of cylinder and the symmetric condition at the middle of cylinder, the homogenous solution can be analytically obtained. The present paper investigates the distribution of the displacement and the stress for different values of non-homogenous index. The axial distribution of the axial displacement, radial displacement, shear stress and the axial stress of cylinder can be presented as the important results of this paper. Calculation of the stress concentration factor due to end effects is another result of the present paper. The obtained results can be analysed for two types of the cylinder with different non homogeneity and temperature distribution.

13/01182 Theoretical modelling of gas flow and filtering of particulates in cracks in containment barriers, and comparison with other theoretical and empirical studies

Han, W. E. *Fusion Engineering and Design*, 2012, 87, (7–8), 1376–1384.

Following earlier publication of a model of crack flow and filtering based on a two-dimensional crack representation, the model has now been improved and submitted to validation by comparison with data from a number of other theoretical and experimental studies. This process has led to improved understanding of gas flow and filtering in real crack geometry and reinforced expectations that the model predictions of barrier filtering capacity will be conservative for realistic containment conditions. This analysis also indicates that, because of drag effects related to the existence of reduced aperture sites, the viscosity limited flow cannot be approximated by the plane Poiseuille model. As a result, theoretical models employing this assumption over-predict measured flow rates by around an order of magnitude. The narrowing of the flow stream at these reduced aperture sites is also found to be a factor which significantly boosts the filtering of particles. As a result of these investigations, there is a strong possibility that all essential elements required have now been identified for a detailed description of aerosol transport through cracks via the laminar flow of a non-condensable carrier gas.

13/01183 Thermodynamic time invariances for dual kinetic experiments: nonlinear single reactions and more

Constales, D. *et al. Chemical Engineering Science*, 2012, 73, 20–29.

For dual kinetic experiments, i.e. experiments performed in batch or steady-state plug flow reactors from reciprocal initial conditions, thermodynamic (space-)time invariances for all reversible single reactions of the first and second order have been found explicitly. In all analysed cases, quotient-like functions of concentrations can be defined which equal the equilibrium constant of the reaction during the whole course of the experiment, and not only at the end, i.e. under equilibrium conditions. The obtained invariances can be used as simple fingerprints for distinguishing the types of reactions. For multistep reactions: (a) a similar invariance was obtained for the two-step catalytic reaction (single route complex reaction) under pseudo-steady-state assumption; (b) for the two-step non-steady-state reaction, an approximation for the thermodynamic invariance was found to be valid in two domains, (1) at the very beginning of the reaction and (2) at the end of the reaction, near equilibrium conditions. The authors hypothesize that such two-domain validity of the thermodynamic invariance is a general feature of dual kinetic experiments performed in complex chemical systems.

13/01184 Threshold length for maximal reaction rate in catalytic microchannels

Mathieu-Potvin, F. and Gosselin, L. *Chemical Engineering Journal*, 2012, 188, 86–97.

This paper addresses the fundamental problem of maximizing the reaction rate of a channel reactor with catalyst on its boundaries by varying its aspect ratio L/H. The volume, pressure drop, amount of catalyst and catalyst surface density of the channels were constrained. The expression of the reaction rate in the limits of small, moderate and large L/H values were obtained by scale analysis. A distinct behaviour appeared for each of these three geometrical limits: a kinetic controlled regime, an external diffusion controlled regime, and a regime limited by fluid flow rates. From this scale analysis, the authors predicted analytically that the length can be varied so as to increase the rate of reaction of a catalytic channel, up to a threshold value from which further change of the geometry does not alter significantly the reaction rate. Intersections of the three reaction rate expressions provided estimates for the maximal reaction rate and for the threshold lengths, as a function of the Bejan number, the Schmidt number and a catalyst number. Finally, CFD simulations of the channel reactors were performed, and numerical parametric studies agreed well with the estimated equations for the threshold L/H values. Correlations based on the numerical data are proposed for the design of catalytic channel reactors.

13/01185 Ultrafast X-ray computed tomography for the analysis of gas–solid fluidized beds

Bieberle, M. *et al. Chemical Engineering Journal*, 2012, 189–190, 356–363.

Gas–particle flow in fluidized beds is generally complex and difficult to observe. But exact information on voidage distribution and solid transport is urgently needed for assessment, monitoring, modelling, and optimization of fluidized bed operation. So far, there was a lack of suitable measurement and imaging techniques to disclose the complex flow structures in fluidized beds with high spatial and temporal resolution. The ultrafast X-ray computed tomography technique, which has been developed in recent years, is superior for such types of multiphase flows and its performance for the analysis of fluidized beds has been demonstrated in this study. Spatial resolution of two millimetres and temporal resolution of several thousand cross-sectional images per second allow at the same time imaging and analysis of voidage structures as well as single particle movement. In this study, the capability of imaging fluidized bed behaviour at different column diameters and gas flow rates has been analysed.

13/01186 Uncertainty quantification in neutron transport with generalized polynomial chaos using the method of characteristics

Ayres, D. A. F. *et al. Annals of Nuclear Energy*, 2012, 45, 14–28.

Polynomial chaos expansion has been used to solve the mono-energetic stochastic neutron transport equation with the spatial and angular components discretized using the step-characteristics method. Uncertainties were assumed to arise purely from the material cross-sections and a novel method for treating uncertainties in discrete, uncorrelated, material regions has been proposed. The method is illustrated by numerical and Monte Carlo simulation of the mean, variance and probability density of the scalar flux for the fixed source Reed cell problem and a critical benchmark in one dimension. For the case of the critical benchmark, the results from the Newton–Krylov root finding method were compared to that of the stochastic collocation method. No benefit in the extra computation of using the Newton–Krylov method was found.

Fuel cell technology

13/01187 A novel sediment microbial fuel cell with a biocathode in the rice rhizosphere

Chen, Z. *et al. Bioresource Technology*, 2012, 108, 55–59.

Wetland plants possess the unique ability to release oxygen as well as organic matter into the rhizosphere. It is understood that microbial fuel cells (MFCs) can use organic matter from plants as key electron donors, but the effect of root excreted oxygen on MFCs is presently unknown. In this study, a novel biocathode was buried in the rice rhizosphere and found to be capable of delivering electrons to root excreted oxygen for oxygen reduction reactions. The voltages between electrodes in the rhizosphere and bulk soil were found to increase initially, but dissipate after approximately 1 month. Results from the MFC and oxygen microelectrode experiments indicated that the oxygen efflux rate from rice roots was dependent on the root maturity. Furthermore, the excreted oxygen from wetland plant roots could be used for the construction of highly efficient biocathodes.

13/01188 A review and design of power electronics converters for fuel cell hybrid system applications

Zhang, Z. *et al. Energy Procedia*, 2012, 20, 301–310.

In this paper, an overview of power electronics converters and inverters for fuel cell hybrid power conversion system is given. Based on the previous research carried out at the Electronics Group of the Technical University of Denmark, a topology proposed here is composed of a dual-input DC–DC converter and three-level NPC inverter. The system can operate in both the stand-alone and grid-connected modes providing fast dynamic response and high efficiency. The benefits of using super-capacitors have been shown clearly in the improved transient response compared to a system with no energy storage elements. Hence, the proposed topology can also be adopted in the applications, such as hybrid electrical vehicles, uninterruptable power supply and PV generation systems. Further research will analyse hybrid energy storage solutions with three or more in converter ports.

13/01189 Discrete approach for flow field designs of parallel channel configurations in fuel cells

Wang, J. and Wang, H. *International Journal of Hydrogen Energy*, 2012, 37, (14), 10881–10897.

It is the major challenge to transform a laboratory scale production of fuel cells to an industrial scale one and to meet the requirements of throughput, operating life, low cost, reliability and high efficiency in R&D of fuel cells. Designs of uniform flow distribution are central to upscale fuel cells as well as to tackle critical issues of water, thermal and current management. However, in spite of the growing appreciation of designs of uniform flow distribution, there is little or no practical solution to ensure a uniform flow distribution across channels of a cell and cells of a stack in designs of flow fields. The purpose of this paper was to develop a discrete approach to find a design that met requirements of flow distribution uniformity and pressure drop in parallel channel configurations with Z-type arrangement through adjustments of configurations and normalized structural parameters. Variation of the frictional and the momentum coefficients with flow velocities was incorporated into the flow distribution equation to improve modelling accuracy. The authors also developed procedure, measures and guideline for the designs of flow distribution and pressure drop to bridge knowledge gap between the generalized theory and industrial applications. The results showed that the present approach could provide the practical guideline to evaluate quantitatively performance of different layout configurations, structures, and flow conditions.

13/01190 Evaluation of potato-processing wastewater treatment in a microbial fuel cell

Durruty, I. *et al. Bioresource Technology*, 2012, 105, 81–87.

Wastewaters from potato-processing industries have been traditionally treated by a sequence of steps that include the production of methane as the anaerobic one. This work explores the feasibility of replacing or supplementing methanogenesis with the emerging technology of microbial fuel cells (MFCs). Electricity producing biofilms have been enriched from a real anaerobic sludge, and the conversion of potato-processing wastewater into electricity has been studied. When tested as a single treatment step, MFCs were able to process the wastewater with high COD removal but with low energetic conversion efficiency. On the other hand, as a complimentary step for methanogenesis, they improved conversion efficiency and significantly reduced the organic matter load of the final effluent. These results point at the combination of the energetic yield of methanogenesis and the improved COD removal of the electricity producing treatment as the implementation choice.

13/01191 Microstructural and high-temperature mechanical characteristics of nickel oxide/zirconia composites for solid oxide fuel cells

Oliva-Ramírez, M. *et al. Fuel Processing Technology*, 2012, 103, 45–50.

NiO/8YSZ (8 mol% Y_2O_3-stabilized ZrO_2) composites with different NiO contents (10, 20 and 40 mol%) have been fabricated by a conventional route of mechanical mixing of NiO and 8YSZ powders and sintering at 1500 °C for 10 h in air. The resulting microstructures have been characterized by electron microscopy. In 10 and 20 mol% NiO/8YSZ, the composite is formed by isolated NiO particles surrounded by zirconia matrix grains; this phase is interconnected in the 40 mol% NiO/8YSZ composite. Mechanical tests at constant strain rate and at constant load were conducted on these materials at temperatures of up to 1350 °C. Different behaviours were found depending on the percolation of the NiO phase. Microstructural observations after deformation are essential to understand the overall mechanical behaviour of the composites.

13/01192 Mixotrophic operation of photo-bioelectrocatalytic fuel cell under anoxygenic microenvironment enhances the light dependent bioelectrogenic activity

Chandra, R. *et al. Bioresource Technology*, 2012, 109, 46–56.

Electrogenic activity of photo-bioelectrocatalytic /photo-biological fuel cell (PhFC) was evaluated in a mixotrophic mode under anoxygenic microenvironment using photosynthetic consortia as biocatalyst. An acetate rich wastewater was used as anolyte for harnessing energy along with additional treatment. Mixotrophic operation facilitated good electrogenic activity and wastewater treatment associated with biomass growth. PhFC operation documented feasible microenvironment for the growth of photosynthetic bacteria compared to algae which was supported by pigment (total chlorophyll and bacteriochlorophyll) and diversity analysis. Pigment data also illustrated the association between bacterial and algal species. The synergistic interaction between anoxygenic and oxygenic photosynthesis was found to be suitable for PhFC operation. Light dependent deposition of electrons at electrode was relatively higher compared to dark dependent electron deposition under anoxygenic condition. PhFC documented for good volatile fatty acids removal by utilizing them as electron donor. Bioelectrochemical behaviour of PhFC was evaluated by voltammetric and chronoamperometry analysis.

13/01193 Modeling of an integrated two-stage biomass gasifier and solid oxide fuel cell system

Colpan, C. O. *et al. Biomass and Bioenergy*, 2012, 42, 132–142.

A new conceptual integrated two-stage biomass gasifier and solid oxide fuel cell (SOFC) system is proposed and a multi-physics model for predicting the performance of this system is developed. A method coupling the modelling equations of a quasi-2D model for SOFC, a 1D model for pyrolysis reactor, and 0D model for the remaining components is applied. Several parametric studies are conducted using the model developed. With the main objective of operating this system being maximizing the net power output, the results for the parametric studies conducted show that the number of SOFC stacks, the mass ratio of air to steam entering the gasifier, and the temperature of the pre-heated air entering the gasifier should be taken as high as possible; whereas the moisture ratio of the wet biomass should be minimized; and there is an optimum point for the rotational speed of the pyrolysis reactor. For the considered input data and the range of parameters studied, the maximum net power output of the system is found to be 93 kW. At this condition, the useful heat output, the electrical efficiency of the system, and the fuel utilization efficiency are calculated as 71 kW, 25%, and 44%, respectively.

13/01194 Numerical study of the effect of the inlet pressure and the height of gas channel on the distribution and consumption of reagents in a fuel cell (PEMFC)

Zeroual, M. *et al. Energy Procedia*, 2012, 18, 205–214.

Proton exchange membrane fuel cell (PEMFC) engines can potentially replace the internal combustion engine for transportation because they are clean, quiet, energy efficient, modular, and capable of quick start-up. Since a PEMFC simultaneously involves electrochemical reactions, current distribution, hydrodynamics, multicomponents transport, and heat transfer, a comprehensive mathematical model is needed to gain a fundamental understanding of the interacting electrochemical and transport phenomena and to provide a computer-aided tool for design and optimization of future fuel cell engines. This paper analyses the effects of inlet pressure and channel height on the distribution and consumption of reagents. The gas flow is assumed laminar, unsteady, isothermal and incompressible, flow fields of the anode and cathode sides are modelled as straight channels. The equations of conservation of mass, momentum and species are developed. A program based on the finite volume method was performed to simulate the system of equations governing the phenomenon. The simulation results show that increasing the inlet pressure will improve consumption of reagents and more homogeneous distribution. The effect of channel height on the consumption of reagents is such that, if the height is smaller it is noticed that there is an increased consumption of species and consequently an increase in water production. Channels with smaller heights have shown a higher concentration of oxygen and hydrogen. The effect of height is more important for a higher pressure inlet.

13/01195 Polymer composites bipolar plates for PEMFCs

Planes, E. *et al. Energy Procedia*, 2012, 20, 311–323.

In order to improve their commercial liability, many scientific and technological efforts are being performed on fuel cell systems. The bipolar plates represent a major part of the stack at about 80% of the total weight and 30–40% of cost. This paper provides a state-of-the-art review of the current development, manufacturing and structure–property relationship of polymer composites designed for bipolar plate applications. Both thermoset resins and thermoplastics were considered and combined to many different carbon fillers: graphite (Gr), carbon fibres (CF), carbon black (CB) and carbon nanotubes (CNT). In order to optimize the two main requirements (electrical and mechanical properties) of composites used for the fabrication of bipolar plates, the flexural strength has been represented as a function of the in-plane conductivity. Most of studied composites have electrical properties required by the application. Nevertheless, the mechanical properties mostly remain below the set of requirements. Consequently it seems to be difficult to obtain a good balance of electrical and mechanical properties. The first way to improve the electrical properties of these composites is to increase the carbon filler content. This strategy is however limited by the wetting problem and the loss in flexural strength that accompanies it. Nevertheless there is another way sparsely studied in the literature, which consists in optimizing the mix of carbon fillers in the composite. This solution seems to give interesting results since the composites filled with different carbon fillers (Gr-CB, Gr-CF, Gr-CNT, Gr-CB-CF) have better mechanical properties than the others composites filled with one carbon filler (Gr). For this type of composites, the graphite must be incorporated as a primary component, because of its high electrical conductivity. In addition, due to its micrometre size, low specific surface area and an aspect ratio close to one, it can be incorporated at high filler content. Then another carbon filler can be added to the formulation. Because of the pore formation in the accumulation of one kind of filler, the pore volume can be reduced by adding smaller particles. This way increases conductive paths and the composite becomes less resistive, but the porosities formation is limited, inducing an improvement of mechanical properties. Carbon black, carbon fibres or carbon nanotubes can be added in addition to graphite, the last two also inducing better mechanical properties. These systems are sparsely studied and an optimization of these formulations and more particularly of the carbon filler choice and their respective proportions will be necessary to reach the two main requirements of bipolar plates.

13/01196 Processing of Foturan® glass ceramic substrates for micro-solid oxide fuel cells

Tölke, R. *et al. Journal of the European Ceramic Society*, 2012, 32, (12), 3229–3238.

The microfabrication of Foturan® glass ceramic as a potential substrate material for micro-solid oxide fuel cells (micro-SOFC) was investigated. Foturan was etched in 10% aqueous hydrofluoric (HF) acid solution at 25 °C with a linear rate of $22 \pm 1.7\,\mu$m/min to create structures with an aspect ratio of 1:1 in 500 μm-thick Foturan substrates for micro-SOFCs. The concentration of the HF etchant was found to influence the etching rate, whereas the UV-exposure time creating nuclei in the glass for subsequent crystallization of the amorphous Foturan material had no significant influence on the etching rates. The surface roughness of the crystallized Foturan® was determined by the crystallite size in the order of 10–15 μm. Free-standing micro-SOFC membranes consisting of a thin film Pt cathode, an yttria-stabilized-zirconia electrolyte and a Pt anode were released by HF etching of the Foturan substrate. An open-circuit voltage of 0.57 V and a maximum power density of 209 mW/cm^2 at 550 °C were achieved.

13/01197 Recent advances in passive and semi-passive direct methanol fuel cells

Faghri, A. *et al. International Journal of Thermal Sciences*, 2012, 62, 12–18.

This paper discusses many recent advances in experimental and numerical studies on methanol supply and water management systems of direct methanol fuel cells (DMFCs) using high concentration including neat methanol. More fundamental and research is required to make the DMFC technology more competitive in the portable and miniature power market. Numerical studies such as a more appropriate kinetics for the methanol oxidation when high concentration methanol is in the catalyst surface, the capillary pressure for the two-phase flow inside the porous media, and the pore-level direct numerical simulation require further investigation. Issues such as durability and cost of the system should be significantly improved in the near future.

13/01198 Simulation of an innovative flow-field design based on a bio inspired pattern for PEM fuel cells

Roshandel, R. *et al. Renewable Energy*, 2012, 41, 86–95.

Proton exchange membrane (PEM) fuel cell performance is directly related to the bipolar plate design and their channels pattern. Power enhancements can be achieved by optimal design of the type, size, or patterns of the channels. It has been realized that the bipolar plate design has significant role on reactant transport as well as water management in a PEM fuel cell. Present work concentrates on improvements in the fuel cell performance by optimization of flow-field design and channels configurations. A three-dimensional, multi-component numerical model of flow distribution based on Navier–Stokes equations using individual computer code is presented. The simulation results showed excellent agreement with the experimental data in previous publications. In this paper, a new bipolar plate design inspired from the existed biological fluid flow patterns in the leaf is presented and analysed. The main design criteria in this research are based on more uniform velocity distribution and more homogeneous molar spreading of species along the flow channels and also higher voltage and power density output in different current densities. By developing a numerical code it was found that the velocity and pressure profiles on catalyst surface are much more uniform, reactant concentration on catalyst surface is very more homogeneous and the power density is higher than parallel and serpentine flow channels up to 56% and 26%, respectively.

13/01199 The effect of the stabilizer on the properties of a synthetic Ni_{core}–Pt_{shell} catalyst for PEM fuel cells

Bhlapibul, S. *et al. Renewable Energy*, 2012, 41, 262–266.

The core–shell structure of Ni_{core}–Pt_{shell} nanoparticles (NPs) was synthesized by a polyol method using 1,2-propanediol. The effect of using a different stabilizer, namely either polyvinylpyrrolidone or oleic acid, was investigated. The results revealed that the two stabilizers differentially affected the crystal structure of the Ni core metal, the particle size and the metal composition of the Ni_{core}–Pt_{shell} NP catalysts. The properties of the catalysts were tested by cyclic voltammetry and linear sweep voltammetry. The Ni_{core}–Pt_{shell} catalyst formed with PVP as the stabilizer gave a higher EAS value, in accord with its smaller particle size, than that formed with oleic acid as the stabilizer. There was no significant difference in the limiting current density of the Ni_{core}–Pt_{shell} catalysts when using the two different stabilizers.

13/01200 Thermal and electrical performance of an alkaline fuel cell

Verhaert, I. *et al. Applied Thermal Engineering*, 2012, 40, 227–235.

Fuel cells have interesting prospects to integrate in alternative energy systems. Alkaline fuel cells have the potential to be manufactured at low cost, as they do not require noble materials for catalysts. To analyse the thermal-physical behaviour of an alkaline fuel cell (AFC), allowing a well-designed integration in a new energy system, a heat and performance study is performed on the AFC stack. An outlook is presented of the different electrical and thermal power outputs and how they can be influenced by the main operating parameters. This will enable the integration of all these power outputs in an optimized energy system. To optimize stack performance, taking both electrical and thermal performance into account, an evaluation method, based on primary energy savings, is presented. Finally, a parameter study is performed, which will enable an improved system design or control strategy for an AFC-based CHP-unit. Most of these improvements are found in a reduction of transmission losses and by increasing input air temperature and humidity, resulting in both higher electric and thermal performance.

13/01201 Zeolite applications in fuel cells: water management and proton conductivity

Han, W. *et al. Chemical Engineering Journal*, 2012, 187, 367–371.

Zeolites are increasingly used in fuel cell, from fuel conversion and conditioning to membrane additives as well as support for electrocatalysts. Zeolites' ionic conductivity and capacity for water adsorption and retention were exploited to create zeolite and zeolite-PFSA proton conducting membranes for PEMFC. HZSM-5 micromembranes of different Si/Al ratios (from ∞ for Sil-1 to 30) were fabricated in a regular array on silicon followed by assembly and test for fuel cell performance. HZSM-5 with high aluminium content exhibits good proton conductivity and better PEMFC performance that approaches that of Nafion MEA. A rational approach in the design of structured HZSM-5-PFSA composite membrane was demonstrated. The PFSA was confined in subnanolitre volumes within zeolite sleeves to obtain self-humidifying membrane and enhanced PEMFC performance (i.e. up to nine-fold in MPD) at elevated temperatures (i.e. up to 100 °C) and dry conditions. Higher water retention and improved membrane thermomechanical properties are believed to be responsible.

15 ENVIRONMENT

Pollution, health protection, applications

13/01202 A preliminary investigation of unintentional POP emissions from thermal wire reclamation at industrial scrap metal recycling parks in China

Nie, Z. *et al. Journal of Hazardous Materials*, 2012, 215–216, 259–265.

Thermal wire reclamation is considered to be a potential source of unintentional persistent organic pollutants (unintentional POPs). In this study, unintentional POP concentrations, including PCDD/Fs, dioxin like PCBs (dl-PCBs), polychlorinated naphthalenes (PCNs), hexachlorobenzene (HxCBz) and pentachlorobenzene (PeCBz), were quantified in flue gas and residual ash emissions from thermal wire reclamation at scrap metal dismantling parks in Zhejiang Province, China. The total average TEQ emissions of the investigated unintentional POPs from flue gas and residual ash in two typical scrap metal recycling plants ranged from 13.1 to 48.3 ng TEQ $N\,m^{-3}$ and 0.08 to 2.8 ng TEQ g^{-1}, respectively. The dominant PCDD/F congeners were OCDD, 1,2,3,4,6,7,8-HpCDD, OCDF and 1,2,3,4,6,7,8-HpCDF, while PCB-126 and PCB-169 were the main contributors to the toxicity of the dl-PCBs. There were clear differences in the distribution dl-PCBs congeners contributing to the TEQ concentrations in the flue gas samples from the two plants. The PCN TEQs were dominated by PCN-66/67 and PCN-73. Although thermal wire reclamation in incinerators has been proposed as an alternative to open burning, there are still considerable environmental risks associated with regulated incinerators, and unintentional POP emissions from thermal wire reclamation sites need to be controlled by local government agencies.

13/01203 A study on air pollutant dispersion with bimolecular reactions in urban street canyons using large-eddy simulations

Kikumoto, H. and Ooka, R. *Journal of Wind Engineering and Industrial Aerodynamics*, 2012, 104–106, 516–522.

Large-eddy simulations (LESs) were performed on the reactive air pollutant dispersion in three types of urban street canyons that had various roof-height levels. Line sources that emit nitrogen monoxide (NO) were set on the bottom of the canyon space in each case. NO dispersed on the cavity eddy and reacted with ozone included in the free stream. The reactivity of air pollutants and the roof heights had a considerable influence on the concentrations of the pollutants inside street canyons. Deeper canyon spaces weakened the ventilation efficiency for pollutants generated inside the canyon. In contrast, variations in the roof height improved the ventilation efficiency. However, in terms of pollutants that came from outside the canyon, the concentration was the lowest for the case with the highest aspect ratio because of the effluent reactions that occurred during retention inside the canyon space. The correlation of the reactors' concentrations was also inspected to reveal the influence of the turbulent nature of the atmosphere on the reaction rate. The correlation had a magnitude of more than 5% to 10% of the total reaction rate inside the street canyons, and it could reach 40% at the maximum in the case with an aspect ratio of 2.0.

13/01204 Assessment of environmental hazards at abandoned mining sites: a case study in Sardinia, Italy

Cidu, R. *et al. Applied Geochemistry*, 2012, 27, (9), 1795–1806.

In the last two centuries, several Pb–Zn mines were active in the Rio Mannu basin near Narcao (south-west Sardinia, Italy), but are now abandoned. These abandoned mines pose a serious risk to the population and required an assessment of the hazard sources and the contaminant pathways in the area. The characterization plan of the Rio Mannu basin was carried out according to Italian protocols. Specifically, samples of soil, stream sediment, fine-grained ore-processing waste (from washery and flotation processes), surface water and groundwater have been analysed in order to assess the levels of contamination in each mine area and the risks in the plains surrounding the site. Several potential chemical contaminants were considered both in solid materials and water samples. The Rosas mine was recognized as the most contaminated area in the basin, due to the presence of a large tailing pond, some fine-grained waste piles and two mine adits with concentrations of the toxic elements As, Cd, Cu, Pb, Sb and Zn exceeding Italian regulatory standards. The dispersion of contaminants occurs downstream from the small stream draining the area. In case of heavy rain the runoff into the streamlet transports the contaminated material far into the plain. The results of this study show that the characterization plan is a relatively cheap tool for establishing mitigation actions, prior to the realization of a complete, and usually expensive, remediation project at abandoned mine sites. Urgent recommended actions in the Rio Mannu basin include the treatment of the adit water prior to its discharge into the Rio Barisonis; the construction of drainage barriers on waste piles to reduce runoff and solid transport into the Rio Barisonis; the consolidation of the earthen dam containing the tailing pond of Rosas to avoid the deepening of erosion furrows that may threaten its stability.

13/01205 Assessment of hygrothermal performance and mould growth risk in ventilated attics in respect to possible climate changes in Sweden

Nik, V. M. *et al. Building and Environment*, 2012, 55, 96–109.

Most of the last 20 years in Sweden have been mild and wet compared to the 1961–1990 climate reference period. After a few relatively cold years in the mid-1980s, practically all years have been warmer than the preceding 30 years average. During the indicated period, an increase of moisture-related problems (mould growth) was observed in ventilated attics, a moisture sensitive building part. This work investigates hygrothermal performance of ventilated attics in respect to possible climate change. Hygrothermal simulations of attics were performed numerically in Matlab. Four attic constructions are investigated – a conventional attic and three alternative constructions suggested by practitioners. Simulations were done for the period of 1961–2100 using the weather data of RCA3 climate model. Effects of three different emissions scenarios are considered. Hygrothermal conditions in the attic are assessed using a mould growth model. Based on the results the highest risk of mould growth was found on the north roof of the attic in Gothenburg, Sweden. Results point to increment of the moisture problems in attics in future. Different emissions scenarios do not influence the risk of mould growth inside the attic due to compensating changes in different variables. Assessing the future performance of the four attics shows that the safe solution is to ventilate the attic mechanically, though this solution inevitably requires extra use of electrical energy for running the fan. Insulating roofs of the attic can decrease the condensation on roofs, but it cannot decrease the risk of mould growth considerably, on the wooden roof underlay.

13/01206 Automating HAZOP studies using D-higraphs

Rodríguez, M. and de la Mata, J. L. *Computers & Chemical Engineering*, 2012, 45, 102–113.

This paper presents the use of D-higraphs to perform HAZOP studies. D-higraphs is a formalism that includes in a single model the functional as well as the structural (ontological) components of any given system. A tool to perform a semi-automatic guided HAZOP study on a process plant is presented. The diagnostic system uses an expert system to predict the behaviour modelled using D-higraphs. This work is applied to the study of an industrial case and its results are compared with other similar approaches proposed in previous studies. The analysis shows that the proposed methodology fits its purpose enabling causal reasoning that explains causes and consequences derived from deviations, it also fills some of the gaps and drawbacks existing in previous reported HAZOP assistant tools.

13/01207 Carbon sequestration, optimum forest rotation and their environmental impact

Kula, E. and Gunalay, Y. *Environmental Impact Assessment Review*, 2012, 37, 18–22.

Due to their large biomass forests assume an important role in the global carbon cycle by moderating the greenhouse effect of atmospheric pollution. The Kyoto Protocol recognizes this contribution by allocating carbon credits to countries which are able to create new forest areas. Sequestrated carbon provides an environmental benefit thus must be taken into account in cost–benefit analysis of afforestation projects. Furthermore, like timber output carbon credits are now tradable assets in the carbon exchange. By using British data, this paper looks at the issue of identifying optimum felling age by considering carbon sequestration benefits simultaneously with timber yields. The results of this analysis show that the inclusion of carbon benefits prolongs the optimum cutting age by requiring trees to stand longer in order to soak up more CO_2. Consequently this finding must be considered in any carbon accounting calculations.

13/01208 Constructivism scenario evolutionary analysis of zero emission regional planning: a case of Qaidam Circular Economy Pilot Area in China

Liu, D. *et al. International Journal of Production Economics*, 2012, 140, (1), 341–356.

The concept of zero emission contributes significantly to sustainable development. China is planning to build a circular economy pilot area with zero emissions in the Western Qaidam Basin. The paper discusses some theoretical and practical issues in the regional planning. In particular, the paper proposes a constructivism scenario evolutionary analysis based on the bargaining games among the involved stakeholders, which embodies the harmonic society criteria in regional plannings. Then, the paper applies the scenario evolutionary analysis method to the multi-objective programming model of the Qaidam Circular Economy Pilot Area, where the objective of environmental pollution minimization can be converted into constraint conditions. Therefore, the problem is converted into the a single objective mixed-integral programming model of the maximal profit under various constraint conditions including natural resources, environment capacity, and social and economic factors, etc. Furthermore, the model provides solutions to the optimal expected output levels of main chemical products and minimal quantity of pollution treatment facilities according to the optimal scenario evolutionary path which embodies the self-purification emission with moderate resource exploitation. The results of the paper will have important policy implications to the regional development planning in China.

13/01209 Contaminant transport through the garage–house interface leakage

Nirvan, G. *et al. Building and Environment*, 2012, 56, 176–183.

Many contaminants in the living space of a house, such as carbon monoxide, benzene, toluene, and ethylbenzene, originate from attached garage. As more airtight and energy-efficient houses are designed and constructed, these contaminants may be retained in indoor air for a longer period of time, jeopardizing the occupants' health. In this study, CONTAM, a multi-zone model, is employed to analyse the effect of garage–house interface on the contaminant transport from an attached garage to the living space. Parametric studies of two buildings are carried out to investigate the effect of ventilation on the transport of contaminant from the garage to living space, based on experimental data of five effective leakage areas of a typical garage–house interface. The results show high concentration of indoor pollutants for typical leaky garage–house interface. Parametric simulations also indicate that the improper design of mechanical exhaust systems can cause higher infiltration of contaminants from the garage to the house, resulting in higher indoor air pollution concentration.

13/01210 Decentralization and participation in integrated coastal management: policy lessons from Brazil and Indonesia

Wever, L. *et al. Ocean & Coastal Management*, 2012, 66, 63–72.

Indonesia and Brazil, two large countries with long coastlines, have seen dramatic political changes over past decades. The new constitution of 1988 in Brazil and the reform movement of 1998 in Indonesia both marked the beginning of a new political era in the respective countries. An important pillar of this was the decentralization of authority. At the same time, the notion of integrated coastal management found its way into national legislation and policies. Key terms during these new eras in both Brazil and Indonesia are decentralization, participation, democratization and, in the context of coastal management, integration. Despite the enactment of promising new laws and policies, and despite local examples of success, implementation still faces a number of challenges in both countries. Inefficiencies and weaknesses of the institutional and legal frameworks have resulted in local mismanagement and misappropriation, a high degree of non-compliance, conflicts between resource users and tension and mistrust between different levels and sections of government. Moreover, the disempowered situation of poorer local ecosystem users largely continues. The authors argue here that for coastal management to become socially more just and environmentally more benign, local communities need to be better informed, capacitated and officially supported in their quest to protect the ecosystems which their livelihoods depend on. Local ecosystem users' social energies and capacities may be essential to respond to ecosystem stakeholders which do not share local ecosystem users' sustainability agendas.

13/01211 Effect of CO_2 capture on the emissions of air pollutants from industrial processes

Kuramochi, T. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 310–328.

This study assesses whether the deployment of CO_2 capture technologies in the European industrial sector would result in significant changes in the emissions of air pollutants (NO_x, SO_2, PM, and NH_3) in the short term. The industrial sectors investigated were: cement, petroleum refineries, and iron and steel. The analysis included onsite emissions and changes associated with grid electricity consumption due to CO_2 capture. Post-combustion capture using monoethanolamine (MEA) was considered for the cement sector and petroleum refineries, and top gas recycling blast furnace (TGRBF) with vacuum-pressure swing adsorption (VPSA) for the iron and steel sector. The results show that when all three industrial sectors in the EU-27 are fully equipped with CO_2 capture, industrial SO_2 emissions in the EU-27 may decrease by 40–70% whereas NH_3 emissions may increase by 120–520% (equivalent to 2–8% of total European emissions). The large increase in NH_3 emissions is due to the degradation of MEA. Cement and petroleum refineries account for nearly all these changes. The results also show limited impact (within ±10% of EU-27 industrial emissions) on NO_x and PM emissions. Emission changes due to electricity import/export are found to be equally important as onsite emission changes. For the iron and steel sector, the changes in National Emissions Ceilings Directive (NECD) emissions are found to be limited for the selected CO_2 capture technique under conservative assumptions. However, the changes in the NECD emissions could vary largely depending on how the steel mill will adapt and operate their coke oven batteries that supply the coke to the blast furnace.

13/01212 Effect of quantity and composition of waste on the prediction of annual methane potential from landfills

Cho, H. S. *et al. Bioresource Technology*, 2012, 109, 86–92.

A study was conducted to investigate the effect of waste composition change on the methane production in landfills. An empirical equation for the methane potential of the mixed waste is derived based on the methane potential values of individual waste components and the compositional ratio of waste components. A correction factor was introduced in the equation and was determined from the BMP and lysimeter tests. The equation and LandGEM were applied for a full size landfill and the annual methane potential was estimated. Results showed that the changes in quantity of waste affected the annual methane potential from the landfill more than the changes of waste composition.

13/01213 Environmental assessment of advanced partitioning, transmutation, and disposal based on long-term risk-informed regulation: PyroGreen

Jung, H. S. *et al. Progress in Nuclear Energy*, 2012, 58, 27–38.

The safety of spent nuclear fuel (SNF) storage has become one of the major issues of nuclear power plant operation. Direct disposal and recycling have both been criticized by the general public due to uncertainty of the long-term safety of SNF and high-level waste (HLW) repositories. To meet the goal of sustainable nuclear energy, an innovative recycling approach using pyrochemical partitioning and transmutation termed PyroGreen, which is a conceptually advanced pyrochemical partitioning flowsheet, has been proposed to eliminate the need for HLW repositories. From the previous partitioning process, PyroGreen uses a combination of hull electrorefining, reductive extraction, and selective oxidation to further decontaminate SNF and HLW into low- and intermediate-level waste (LILW). This paper examines the long-term environmental performance of a geological repository that houses all of the final PyroGreen-produced wastes while describing the feasibility of PyroGreen partitioning and transmutation. The final PyroGreen wastes are evaluated based on long-term risk-informed criteria: alpha-emitting isotope concentration, heat generation, and radiation dose in the surrounding biosphere. All final wastes arising from PyroGreen are to be disposed of in a geological repository at an intermediate depth, in compliance with new International Atomic Energy Agency safety guide for LILW. Migration assessment found that several long-lived fission products including C-14, Cl-36, Se-79, Sn-125, and I-129 dominate the long-term dose rate, whereas transuranic elements govern the risk of an inadvertent human intrusion scenario. In order to turn entire batches of SNF from 24 light water reactors with 1000 MWe with a design life of 40 years into LILW, the authors determined and compared the required decontamination factors of the key radionuclides for between intermediate-depth and near-surface disposal.

13/01214 Environmental impact assessment of composites containing recycled plastics

Rajendran, S. *et al. Resources, Conservation and Recycling*, 2012, 60, 131–139.

Using recycled plastics can significantly reduce the environmental impacts by avoiding exploration, mining and transportation of natural gas and oil. Adding fibrous reinforcement is a potential way to increase the recycling rate and also to locate high value applications to recycled plastics. The environmental impact assessment has been carried out using life cycle assessment (LCA) approach. The glass fibres and flax fibres were chosen as fibrous reinforcement. The resource depletion potential and global warming potential were evaluated for glass fibre and flax fibre filled recycled plastics and compared with their respective virgin alternatives. The properties of the recycled and virgin composites were estimated from the literatures and semi-empirical models. The resource depletion and global warming were compared at equivalent stiffness's. The results indicate that reinforcing recycled plastics can significantly reduce the resource consumption and global warming in civil and infrastructural applications. However, the composites made from virgin plastics remain a greener and sustainable alternative in the automotive applications.

13/01215 Evaluation of organic waste diversion alternatives for greenhouse gas reduction

Yoshida, H. *et al. Resources, Conservation and Recycling*, 2012, 60, 1–9.

Greenhouse gas (GHG) emission analysis was performed for current and proposed organic waste management practices in the city of Madison, Wisconsin, USA. Aiming for the long-term goal of zero waste, the City of Madison has been looking into an opportunity to divert its organic waste from its landfill. Previous studies suggested that organic waste diversion could result in a GHG emission reduction. Alternative treatment of organic waste would reduce GHG emissions through avoidance of landfill methane emission, nutrient replacement, and energy recovery when anaerobic digestion technologies are employed. However, organic waste diversion requires modification of collection practices and additions to the collection fleet. This would increase the GHG emissions and there is a need to balance emission reductions and the additional costs associated with a new organic waste diversion program. Collection practices are also important for the success of such a project, as it accounts for 83% of current operational cost for managing organic waste. The GHG emissions were quantified using the life cycle assessment (LCA) approach. The current practice of composting of yard waste and direct disposal of other fractions of organic waste into the landfill were estimated to emit 224 kg CO_2-eq./ton of GHG. In contrast with the current practice, four alternatives were assessed in this study: windrow composting, high-solids anaerobic digestion, co-digestion at a large scale industrial waste anaerobic digester facility, and co-digestion at the local wastewater treatment plant. The results show that the co-digestion of source-separated organic waste would achieve the highest GHG emission reduction among the alternatives considered. The results were as follows: 81.5 kg CO_2-eq./ton for windrow composting; −46.0 kg CO_2-eq./ton for a high solids anaerobic digester; −156 kg CO_2-eq./ton for co-digestion with industrial waste; and −189 kg CO_2-eq./ton for co-digestion with sewage sludge. Co-digestion was favoured as it shows the highest GHG emission reduction capacity while saving capital cost by almost half. However, the results of the GHG emission analysis were also affected by several factors external to the technologies chosen, including public participation, collection efficiency of organic waste, and types of waste collected. Based on the findings of this work, the party in charge of the organic waste diversion project should seek opportunities to partner with regional anaerobic digestion projects and local utilities, while continuing with its community outreach efforts.

13/01216 Green occupants for green buildings: the missing link?

Deuble, M. P. and de Dear, R. J. *Building and Environment*, 2012, 56, 21–27.

Green buildings, often defined as those featuring natural ventilation capabilities, i.e. low-energy or free-running buildings, are now at the forefront of building research and climate change mitigation scenarios. This paper follows the results of recent post-occupancy evaluation (POE) surveys within two academic office buildings located in sub-tropical Sydney, Australia. Supplemented with an environmental attitudes questionnaire, based on the 'new ecological paradigm', it was found that occupant satisfaction levels on the POE were positively associated with environmental beliefs. Occupants with higher levels of environmental concern were more forgiving of their building, particularly those featuring aspects of green design, such as natural ventilation through operable windows. Despite their criticisms of the building's indoor environmental quality, the 'green' occupants were prepared to overlook and forgive less-than-ideal conditions more so than their 'brown' (non-green) counterparts. These results support the hypothesis that pro-environmental attitudes are closely associated with the stronger 'forgiveness factor' often observed in green buildings, but the question of causality remains moot.

13/01217 Improved lead recovery and sulphate removal from used lead acid battery through electrokinetic technique

Soundarrajan, C. *et al. Journal of Hazardous Materials*, 2012, 217–218, 452–456.

This paper presents improvement in lead recovery and sulfate removal from a used lead–acid battery (ULAB) through an electrokinetic technique, a process aimed to eliminate environmental pollution that arises due to emission of gases and metal particles from the existing high-temperature pyrometallurgical process. Two different cell configurations, one with a Nafion membrane placed between anode and middle compartments and an agar membrane between cathode and middle compartments and another with only an agar membrane placed between both sides of the middle compartments were designed for the Pb and sulfate separation from ULAB. This paper concludes that the cell with only agar membranes performed better than the cell with Nafion and agar membranes in combinations and also explains the mechanism underlying the chemical and electrochemical processes in the cell.

13/01218 Informed public opinion in the Netherlands: evaluation of CO_2 capture and storage technologies in comparison with other CO_2 mitigation options

de Best-Waldhober, M. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 169–180.

In this study, 995 respondents in a representative sample of the Dutch general population are set in the situation of policymakers: they are faced with the issue of fulfilling the Dutch demand for energy in 2030 in such a way that emissions of carbon dioxide will be reduced by 50%. In the information-choice questionnaire (ICQ) that was developed for this, respondents evaluated information from experts on seven options for CO_2 emission reduction and their consequences. Two carbon dioxide capture and storage (CCS) options were compared to two energy efficiency options, a wind energy option, a biomass energy option, and a nuclear energy option. Results show that people are not that enthusiastic regarding the two CCS options. These are evaluated 5.3 and 5.9 on average on a scale of 1–10 and not often chosen as one of the three preferred options, but they are also rarely rejected. Most of the other options in the questionnaire were evaluated rather positively, except nuclear energy and the more ambitious efficiency option. Analysis shows that the evaluation of the information regarding consequences moderately influences how options are evaluated overall. The results further indicate that the CCS options are evaluated less positively due to the comparison with other options.

13/01219 Institutional pressure and waste reduction: the role of investments in waste reduction resources

Simpson, D. *International Journal of Production Economics*, 2012, 139, (1), 330–339.

The introduction of increased recycling and recovery laws in the European Union and a growing number of countries have forced firms to consider their waste reduction performance. Firms that are unable to understand the complexities of waste recycling and recovery are increasingly at a disadvantage relative to firms that can. Firms for example that do not develop capabilities that support waste recycling must rely on costly third party disposal and treatment options. Identification of beneficial combinations of waste reduction resources however that can be used by firms remains underexplored. In this study, it is proposed that firms' investment in resources that allow them to improve their waste reduction performance has competitive advantage implications. These resources are expected to mediate the relationship between external pressure to reduce waste and firms' waste reduction performance. These resources, such as equipment, personnel or R&D, provide firms with important context-specific capabilities. In this study, the relationship between institutional pressures, waste reduction resources and performance was assessed for a sample of US manufacturers. Study findings indicated that firms' investments in waste reduction resources provided them with significant advantages in the form of increased pollution and cost reduction. The results suggest that waste reduction resources better position firms to predict and effectively respond to institutional pressures. From a policy perspective, the benefits of waste reduction resources can be highlighted and more specific payback calculated for specific resource types. The findings of this study further support the role of resources to environmental performance improvement in the study of sustainable operations.

13/01220 Mine safety information technology in the framework of Digital Mine

Li, C. *et al. Safety Science*, 2012, 50, (4), 846–850.

Digital Mine is a key research domain of Digital Earth. Because of the spatio-temporal, three-dimensional and intrinsically dynamic nature of mine safety management data, it is difficult to make a breakthrough in this domain. As a key part of Digital Mine, the construction of the Digital Mine Safety Management System (DMSMS) pushes Digital Mine a step forward from operation as a mere concept to achievement as a realistic system. In this paper, the technical framework of the DMSMS in the framework of Digital Mine is discussed, including its data, function and application layers. A key technology is then studied in detail that will enable the construction of the three-dimensional geological environment and the visualization and integration of the mine safety data.

13/01221 Non-conventional interfaces for human-system interaction in nuclear plants' virtual simulations

Aghina, M. A. C. *et al. Progress in Nuclear Energy*, 2012, 59, 33–43.

This paper reports recent results achieved in a research and development (R&D) with non-conventional interfaces for human-system interaction in nuclear plants' virtual simulations. This R&D aims at developing applications based on virtual reality technology for simulations toward training, ergonomics evaluation, safety and security purposes in the nuclear engineering field. Two main applications are under development, one comprising a virtual control desk for users' interaction with a computer-based nuclear power plant simulator, and the other comprising multi-user navigation in virtual environments which in turn correspond to nuclear plants and other sites. Non-conventional interfaces mean more friendly and natural human-system interfaces, compared to computer keyboard and mouse, as speech-based command recognition and face tracking. Besides the benefits of using one or other of these non-conventional interfaces, a combination of them could further improve human-system interaction, through exploring each approach's advantages for specific corresponding tasks. A solution adopted for implementation with the navigation in the virtual environments' application is explained. Results are discussed and perspectives are given for future developments.

13/01222 Oligopolies in pollution permit markets: a dynamic game approach

Chung, S. H. *et al. International Journal of Production Economics*, 2012, 140, (1), 48–56.

The authors reconsider the pollution permit concept in a setting extended to include dynamics, spatially diversified firms, and an oligopoly in product markets. The firms can manage their pollution emissions or stocks by (1) buying pollution permits and emitting pollution, (2) shipping pollutants to other nodes and paying such shipping costs, or (3) paying environmental costs to mitigate or recycle pollution. Firms manage these controls strategically to maximize net profits while facing non-cooperative rivals. Within this setting, the authors show that the non-cooperative competition among firms may be represented as a differential variational inequality (DVI) framework. Furthermore, the authors propose decision rules on permit purchase, establish necessary conditions, and prove the existence of solution in the formalism of the DVI. They also show that the DVI can be equivalently converted to a non-linear complementarity problem, and show this problem, despite high dimensions, is efficiently solvable using off-the-shelf software (GAMS with the PATH solver). The authors illustrate this method's feasibility with a computationally intensive numerical example.

13/01223 Radiation impact assessment on wildlife from an uranium mine area

Černe, M. *et al. Nuclear Engineering and Design*, 2012, 246, 203–209.

Uranium mining and milling activities are one of the major causes of radioactive contamination of the environment. Radionuclides, especially uranium decay-chain products, are released from plant wastes into the soil and water and consequently into vegetation where they may accumulate. Transfer of radionuclides thus represents a radiological risk to humans and non-human organisms due to accumulation of radionuclides in target tissues and the consequent ionizing radiation. The uranium mine at Žirovski vrh in Slovenia, which operated from 1985 to 1990, processed about 600,000 t of U-ore. Operational wastes were deposited at the Boršt and Jazbec sites. According to several studies, an environmental radiological risk to biota could be observed at sites exposed to radioactive contamination. A modelling approach can be used to estimate the risk in such areas. The ERICA tool is one of the more widely used models, developed to assess the environmental risk from ionizing radiation to wildlife. In this study, the ERICA Tool was applied for the assessment of the radiation impact on wildlife in the Žirovski vrh influential area. ERICA reference organisms, native plants and aquatic organisms were included in the assessment to screen the risk to different organisms. Total dose rate to organisms were up to 3.49, 33.0 and $2.58\,\mu\mathrm{Gy\,h^{-1}}$ for *Juncus effusus*, lichens and *Austropotamobius torrentium*, respectively. Dose rates to other organisms are also presented and discussed.

13/01224 Research on 10-year tendency of China coal mine accidents and the characteristics of human factors

Chen, H. *et al. Safety Science*, 2012, 50, (4), 745–750.

The trend of coal mine accidents in China over the last 10 years was studied and the human factors in these accidents were analysed by multi-dimensional statistical analysis. The analyses show that the number of major coal mine accidents and the death toll in the accidents were decreasing steadily, while sporadic death accidents still accounted for the largest percentage of deaths. Gas outburst accidents, gas explosion accidents and mine water accidents remained the major part of the whole story and subject to close attention. Among the causes of these accidents, human factors accounted for 94.09%, of which intentional violation, mismanagement and defective design accounted for 35.43%, 55.12% and 3.54%, respectively. Improper operational and management practices in which the safety system, procedures and specifications were neglected or broken were still key roots of Chinese coal mine accidents.

13/01225 Studies on removal of NH_4^+-N from aqueous solution by using the activated carbons derived from rice husk

Zhu, K. *et al. Biomass and Bioenergy*, 2012, 43, 18–25.

Water pollution caused by ammonia nitrogen has attracted a great attention as its toxicity affects both the environment and human health. The objective of this paper was to investigate the adsorption behaviour of NH_4^+-N from aqueous solution by activated carbons prepared from rice husk. The physicochemical properties of the activated carbon were characterized by Brunauer–Emmett–Teller test, Fourier transform infrared spectroscopy and scanning electron microscopy. It was found that the NH_4^+-N adsorption on the rice husk derived carbons was dependent on adsorbent dosage and solution pH. The adsorption kinetics and isotherms of NH_4^+-N by rice husk carbon were also investigated, and good correlation coefficients were obtained for the pseudo-second order kinetic equation. Dubinin–Radushkevitch (D-R) adsorption isotherm model could better describe the adsorption behaviour of NH_4^+-N on the rice husk carbon. Calculated by D-R model, the adsorption course of NH_4^+-N on the rice husk carbon was favoured chemical ion-exchange mechanism. Moreover, the activated carbon adsorbed NH_4^+-N was highly fertilizer conservation especially for the nitrogen element. It was proposed that the amount of removed NH_4^+-N from aqueous solutions would increase evidently treated by rice husk carbon if combined with biological method.

13/01226 The conditions for, and challenges of, adapting England's suburbs for climate change

Williams, K. *et al. Building and Environment*, 2012, 55, 131–140.

This paper outlines the conditions for, and challenges of, adapting suburbs in England for climate change. The paper introduces the 'suburb' as a spatial setting vulnerable to climate change related threats that have been largely absent from previous adaptation studies. It argues that in terms of the impacts of climate change on the daily lives of the UK's population suburban neighbourhoods need far more attention. It sets out a typology of English suburbs (including inner-historic suburbs, pre-war garden suburbs, interwar suburbs, social housing suburbs, car suburbs, and medium-high density suburbs), and argues that these suburbs will experience both gradual changes in climate and extreme events. The changes will have impacts on 'place' and 'people', and modifications to the physical environment to respond to climate change will need to take place if they are to be sustainable in the future. Modifications can be at different scales: home and/or garden and/or neighbourhood. However, whether or not such modifications to the physical environment will be implemented is a function of the 'response capacity' in the suburb: and this is determined partly by the existing physical conditions of the suburb, and partly by economic, governance, knowledge and cultural contexts. The paper describes the conditions that underlie the response capacity in suburbs, and reveals the complexity of attempting to 'climate proof' some of the most established and valued parts of the English urban landscape.

13/01227 The influence of building height variability on pollutant dispersion and pedestrian ventilation in idealized high-rise urban areas

Hang, J. *et al. Building and Environment*, 2012, 56, 346–360.

Studies are still required to understand how rural/marine wind removed ground-level pollutants released uniformly in street networks of high-rise urban areas. The link between building height variability and pollutant removal process still remains unclear. Several idealized urban-like neighbourhoods made of nine- and 18-row small-scale, high-rise square arrays (building width B = street width W, building packing density $\lambda_p = 0.25$) were first numerically studied with a parallel approaching wind and neglecting thermal effects. Normalized pollutant transport rates and pedestrian purging flow rate were applied to quantify the contribution of pollutant removal by mean flow and turbulent diffusion and their net purging capacity. Results show that the prediction of isothermal turbulent flows agreed generally well with wind tunnel data. For nine-row arrays with building height variations (standard deviation of 0–57.1%) and the same average canopy height ($H_0 = 2.33W$), pollutant removal mainly depends on mean flows. Larger standard deviations tend to induce better pedestrian ventilation. In comparison to small and large standard deviations, medium values of 14.3–42.9% may experience smaller purging capacity by horizontal mean flows but significantly enhance that by vertical mean flows. For arrays with uniform heights, lowering aspect ratios ($H/W = 2.33$ and 2.67–1.5) or increasing street lengths (nine- to 18-row) may enhance the contribution of removing pollutants by turbulent diffusions across canopy roofs which may be similarly important as that by mean flows. Although further investigations are still required, this paper clarifies the relationship between building layouts, height variability and removal potential of ground-level pollutants in high-rise urban-like geometries.

13/01228 Upgrading of woody biomass by torrefaction under pressure

Wannapeera, J. and Worasuwannarak, N. *Journal of Analytical and Applied Pyrolysis*, 2012, 96, 173–180.

In this study, the upgrading by torrefaction of leucaena, woody biomass, at 200–250 °C under volumetric pressure up to 4 MPa was examined. It was found that the yield of torrefied leucaena decreased with the increase in torrefaction temperature, whereas at the same temperature the yield of torrefied leucaena increased with the increase in torrefaction pressure. From the elemental analyses, the higher carbon content in torrefied leucaena can be achieved by the rising of torrefaction pressure. As large as 92.6% of carbon was recovered in the torrefied leucaena prepared at 250 °C and 4 MPa. On the other hand, the oxygen content decreased to 31.1% for the leucaena torrefied at 250 °C and 4 MPa. The higher heating value (HHV) of leucaena torrefied at high pressure increased significantly when compared to that of leucaena torrefied at atmospheric pressure. As large as 94.3% of energy yield was achieved with the mass yield of 74.4% for the torrefaction at 250 °C and 4 MPa. From the subsequent pyrolysis and combustion in TGA, leucaena torrefied under pressure showed the difference of weight decreasing curves comparing to that of leucaena torrefied at atmospheric pressure. It was found that the weight of leucaena torrefied at high pressure started to decrease at temperature lower than 200 °C. The char yield at 800 °C for the leucaena torrefied at high pressure increased with the increase in torrefaction pressure. These results suggested that the structure of leucaena was changed by the torrefaction under pressure and the cross-linking reactions during the pyrolysis were enhanced by the pressure during the torrefaction resulting in increase in char yields. The substantial increase in char combustion rate was also found for leucaena torrefied under pressure.

13/01229 Vulnerability assessment of water supply network

Zohra, H. F. *et al. Energy Procedia*, 2012, 18, 772–783.

With global warming, water supply is becoming a problem in areas of the southern hemisphere where rain is decreasing considerably. As a result, preserving such resource is becoming a crucial task facing the authorities. One of the main ways of preservation is making the water pipelines network as safe as possible from any damages involving loss of water around urban areas in particular those situated within areas prone to seismicity. For this purpose, a method to assess the seismic vulnerability of water pipelines was developed and implemented in a geographical information system, allowing larger water supply network to be covered and studied. This method is based on the identification of the parameters that have an influence on the behaviour of pipelines. Each parameter having a coefficient that represent its influence on the behaviour of the structure, the product of these parameters represent the seismic vulnerability of the section pipe under study. As a result, a proposed classification is obtained allowing the determination of a safe section (green colour), an unsafe section (red colour) and an intermediate situation (orange colour). For a proposed application of the method, a case study for a town in suburb of Algiers is presented within this paper. It concerns the town of Blida and the results show that 23% of the pipelines which represent 24.1% of the total length of the network are vulnerable to seismic action so they must be replaced first. In fact about 70% of the network needs renovation; this is in appropriateness with general conclusion of a previous study. Although the framework of this study is common to various models of statistical estimation method, the vulnerability index developed method is an easy way to show the most vulnerable pipe of a supply water network. Despite the fact that the ranges of the classification need to be improved, the proposed classification give satisfaction results according what was observed *in situ*.

13/01230 Willingness to engage in a pro-environmental behavior: an analysis of e-waste recycling based on a national survey of U.S. households

Saphores, J.-D. M. *et al. Resources, Conservation and Recycling*, 2012, 60, 49–63.

Using concepts from environmental psychology and economics, this study investigates US households' willingness to engage in a form of pro-environmental behaviour: recycling electronic waste (e-waste) at drop-off locations. The study relied on a rich dataset from a 2006 national survey of US households ($N = 2136$). The internal variables include a modified version of the new ecological paradigm scale, a moral norm scale based on Schwartz's norm-activation model, and indicators of social pressure for recycling. External variables consist of detailed socio-demographic characteristics. The logit model shows that external variables do not help characterizing people with e-waste recycling experience, except that they tend to have larger families or to be over 60 years old. However, knowing that e-waste contains potentially toxic materials, recycling conventional materials at work or at school, and especially having strong moral norms helps explain e-waste recycling behaviour. Using a generalized ordered logit model, it was found that the most important variables for explaining household willingness to recycle e-waste are internal variables, followed by recycling convenience, knowledge of the potential toxicity of e-waste, prior e-waste recycling experience, as well as gender and marital status; education, age, and ethnicity play only a minor role, while knowledge of e-waste laws, availability of curbside recycling for domestic waste, and income are not statistically significant. The results suggest that e-waste recycling can be stimulated by promoting moral norms, educating the public about the benefits of recycling e-waste, and making e-waste recycling more convenient but other measures will likely be necessary to tackle the e-waste problem.

CO_2, NO_x, SO_2 and particulate emissions

13/01231 A primary method for reducing nitrogen oxides in coal combustion through addition of Bio-CONOx

Poskrobko, S. *et al. Fuel Processing Technology*, 2012, 101, 58–63.

The aim of this paper is to demonstrate an effective primary method for reducing NO_x in coal combustion in a retort underfeed stoker boiler through addition of extracted rapeseed meal, i.e. via co-firing process. It is shown that the additive is characterized by slow thermodecomposition in a high temperature interval associated with a release of considerable amounts of ammonia, light hydrocarbons including methane, active free radicals, ketones, and other nitrogen compounds. Subsequently, as high amount of volatile matter contained in extracted rapeseed meal results in a local deficiency of oxygen, the concentration of NO_x in the exhaust gas is reduced through two combined mechanisms: de-NO_x process as in the SNCR method and reburning. The combustion tests showed that with the increased amount of the additive from around 10% to just over 30% the relative reduction of NO_x emissions grows from about 15% to over 40%. This way one can reduce the NO_x emissions in boilers with heat output up to 10 MW. There exists a number of other biomass species that could presumably behave similarly to extracted rapeseed meal in the combustion process. This whole family of substances has been named Bio-CONOx.

13/01232 Attributing land-use change carbon emissions to exported biomass

Saikku, L. *et al. Environmental Impact Assessment Review*, 2012, 37, 47–54.

In this study, a simple, transparent and robust method is developed in which land-use change (LUC) emissions are retrospectively attributed to exported biomass products based on the agricultural area occupied for the production. LUC emissions account for approximately one-fifth of current greenhouse gas (GHG) emissions. Increasing agricultural exports are becoming an important driver of deforestation. Brazil and Indonesia are used as case studies due to their significant deforestation in recent years. According to this study, in 2007, approximately 32% and 15% of the total agricultural land harvested and LUC emissions in Brazil and Indonesia respectively were due to exports. The most important exported single items with regard to deforestation were palm oil for Indonesia and bovine meat for Brazil. To reduce GHG emissions effectively worldwide, leakage of emissions should be avoided. This can be done, for example, by attributing embodied LUC emissions to exported biomass products. With the approach developed in this study, controversial attribution between direct and indirect LUC and amortization of emissions over the product life cycle can be overcome, as the method operates on an average basis and annual level. The approach could be considered in the context of the UNFCCC climate policy instead of, or alongside with, other instruments aimed at reducing deforestation. However, the quality of the data should be improved and some methodological issues, such as the allocation procedure in multiproduct systems and the possible dilution effect through third parties not committed to emission reduction targets, should be considered.

13/01233 Burnout of soot particles in a two-stage burner with a JP-8 surrogate fuel

Echavarria, C. A. *et al. Combustion and Flame*, 2012, 159, (7), 2441–2448.

This work focuses on the understanding of the oxidation of soot particles which were the result of using a JP-8 surrogate fuel in a two-stage burner. The two-stage system consists of an initial premixed burner where soot was generated with an air/fuel mixture, specifically a JP-8 surrogate (*m*-xylene and *n*-dodecane), under a variety of conditions. Downstream, the soot-laden combustion gases were passed through a second, flat-flame burner where soot was burned out under fuel-lean or slightly fuel-rich conditions. Soot oxidation in the secondary burner was determined by investigating particle size distribution (PSD), flame temperature, gas-phase composition, soot surface area, and soot morphology and nanostructure as a function of the height above the second burner (HAB). Measurements of soot size distribution and number concentration as a function of the HAB under fuel lean (Φoverall = 0.8) and slightly rich (Φoverall = 1.14) conditions showed a decrease in particle mean diameter and a significant increase in number concentration in the region where O_2 concentration decreased. In this region, the effectiveness factor for O_2 was found to be 1, indicating the potential for internal oxygen diffusion and burning. This caused both the breakup of the bridges cementing primary particles and the rupture of the primary particles. Higher in the burner, where modelling suggested the presence of OH*, soot oxidation was attributed to OH* mechanisms which are faster as compared to O_2 oxidation.

13/01234 Characteristics of particles and black carbon emitted by combustion of incenses, candles and anti-mosquito products

Stabile, L. *et al. Building and Environment*, 2012, 56, 184–191.

Indoor combustion sources are of great concern when accurate evaluations of the overall human exposure to particles have to be provided. Even if cooking activity was claimed to be the most emitting source in indoor environments, other indoor activities involving incense, candle and anti-mosquito product combustions can produce high particle concentrations. To this purpose, studies evaluating particulate matter (PM) fraction emission rates from such indoor activities were performed, even if there is still a lack of understanding in terms of particle number and carbonaceous amount (black carbon, BC) carried by particles themselves. The aim of the present study was to characterize the particle emission due to the combustion processes of incenses, candles and anti-mosquito products. Emission factors in terms of number, surface area and PM fraction concentrations were evaluated through a condensation particle counter, a scanning mobility particle sizer, and an aerodynamic particle sizer. Moreover, BC emission factors were measured through an aethalometer. Particles' BC content distribution was also measured proposing an experimental method made up of a particle size classification device connected to an aethalometer. Emission factors due to incenses and anti-mosquito products were higher than 10^{14} part h^{-1} and 48 mg h^{-1} in terms of number and PM_{10} concentrations, respectively. Differently, PM fraction emissions from candle burning were well below 1 mg h^{-1}. Nonetheless, BC emission rate and distribution measurements showed that candle flaming combustion produces mainly carbonaceous particles (BC/PM_{10} ratio higher than 80%). Differently, smouldering combustion processes, like incense and anti-mosquito product combustions, showed a negligible amount of BC.

13/01235 Comparing CO_2 and NO_x emissions from a district heating system with mass-burn waste incineration versus likely alternative solutions – city of Trondheim, 1986–2009

Brattebø, H. and Reenaas, M. *Resources, Conservation and Recycling*, 2012, 60, 147–158.

There is a rapidly growing literature on the environmental performance of waste-to-energy technologies, including the use of waste incineration with heat recovery as integrated part of urban district heating systems. This study highlights findings from some of the recent literature, and carries out a case study for 24 years of operation of a district heating system in Trondheim, Norway. This is a system with heat recovery (not co-generation) from mass-burn incineration of residual (source-sorted) municipal waste, as well as a significant heat input from other energy sources for back-up and peak load demand supply. The use of such additional fuels is common for district heating systems in cold climate, as the solid waste base load is clearly insufficient during cold winter periods. Hence, this study goes beyond a conventional waste-to-energy analysis, addressing the overall combined system of waste treatment and heat supply in an urban area. Life cycle analysis principles are used to determine direct and indirect emissions of CO_2-eq and NO_x from main elements in the combined system. These emissions are compared to a hypothetic scenario with the most likely alternative waste treatment and heat supply technologies during the study period, i.e. since 1986. The paper demonstrates the performance difference of these two cases, clarifies which elements of the combined system are the important ones, and discusses the role of other energy sources than waste. Furthermore, the importance of choices of electricity (El-mix) is demonstrated, comparing average Norwegian, Nordic and European El-mix. Finally, the potential influence of changed calorific value of residual waste is analysed, which is likely to be important in future due to changing policies for source-sorting of municipal waste.

13/01236 CO_2 disposal as hydrate in ocean sediments

Qanbari, F. *et al. Journal of Natural Gas Science and Engineering*, 2012, 8, 139–149.

Reducing carbon dioxide (CO_2) emissions is becoming a significant environmental goal and undertaking worldwide, and is expected to be a major concern in the future. In this regard, sequestration of CO_2 in geological formations is of great interest. However, CO_2 is buoyant under the pressure-temperature conditions of typical geological sites, contributing to the risk of leakage. Storage of CO_2 as hydrate avoids this limitation. Much of the ocean sediments at depths of a few hundred meters below the ocean floor provide appropriate conditions for CO_2 hydrate formation. Furthermore, ocean sediments may provide conditions at which the density of liquid CO_2 is greater than the density of water, making liquid CO_2 gravitationally stable (i.e. non-buoyant). This study investigates storage of CO_2 as hydrate below the ocean floor. The authors identify conditions where the initial pressure-temperature conditions are suitable for CO_2 hydrate formation and demonstrate the effect of changes caused by injection. In particular, the changes in pressure as a result of injection and the increase in temperature due to hydrate formation, both of which could lead to upward movement of CO_2, are investigated. Sensitivity studies are conducted to determine appropriate conditions for large scale CO_2 storage. In particular, the effects of ocean depth and injection depth in the sediment on flow of CO_2 toward the ocean floor are studied. The results of calculations for static conditions and modelling under dynamic conditions show that CO_2 hydrate formation and gravitational stability of CO_2 in the upper parts of the ocean sediments for some areas of the ocean can restrict upwards flow of CO_2 toward the seabed. If the ocean depth and sediment depth for injection of CO_2 are properly chosen, large volumes of CO_2 can be reliably stored in the sediment.

13/01237 Design and scale-up of an oxidative scrubbing process for the selective removal of hydrogen sulfide from biogas

Krischan, J. *et al. Journal of Hazardous Materials*, 2012, 215–216, 49–56.

Reliable and selective removal of hydrogen sulfide (H_2S) is an essential part of the biogas upgrading procedure in order to obtain a marketable and competitive natural gas substitute for flexible utilization. A promising biogas desulfurization technology has to ensure high separation efficiency regardless of process conditions or H_2S load without the use or production of toxic or ecologically harmful substances. Alkaline oxidative scrubbing is an interesting alternative to existing desulfurization technologies and is investigated in this work. In experiments on a stirred tank reactor and a continuous scrubbing column in laboratory-scale, H_2S was absorbed from a gas stream containing large amounts of carbon dioxide (CO_2) into an aqueous solution prepared from sodium hydroxide (NaOH), sodium bicarbonate ($NaHCO_3$) and hydrogen peroxide (H_2O_2). The influence of pH, redox potential and solution aging on the absorption efficiency and the consumption of chemicals was investigated. Because of the irreversible oxidation reactions of dissolved H_2S with H_2O_2, high H_2S removal efficiencies were achieved while the CO_2 absorption was kept low. At an existing biogas upgrading plant an industrial-scale pilot scrubber was constructed, which efficiently desulfurizes $180\,m^3/h$ of raw biogas with an average removal efficiency of 97%, even at relatively high and strongly fluctuating H_2S contents in the crude gas.

13/01238 Emission of NO_x and N_2O from co-combustion of coal and biomasses in CFB combustor

Saikaew, T. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 26–32.

Utilization of biomass in combustion processes is a promising way to reduce net emission of greenhouse gas, e.g. CO_2, to atmosphere. However, biomass is not likely to be successfully employed as a single feedstock due to its low energy density compared to coal. The co-combustion of coal and biomass in a circulating fluidized bed combustor (CFBC) can be employed to address this issue by improving the overall calorific value. This work investigated the influences of different biomass types on CFBC emissions. Sub-bituminous coal along with four biomass types such as palm shell, coconut shell, sawdust and rice husk were employed in study. The results indicated that the temperature profile in the riser was matter relevant to the heating value of fuel mixtures. The co-combustion of coal and palm shell gave the highest average combustion temperature, due to comparable heating value of both fuels. On the other hand, the co-combustion of coal and rice husk, which has relatively lower heating value, gave the lowest temperature. The presence of biomass in combustion was found to lead to a reduction of NO_x and N_2O in flue gas. The fuel-nitrogen content was observed to be a major factor for determining both NO_x and N_2O emission. Moreover, this work exhibited that the injection of secondary air with different position into the riser influenced the NO_x and N_2O concentration in the flue gas.

13/01239 Hazardous gas emissions from the flanks of the quiescent Colli Albani volcano (Rome, Italy)

Carapezza, M. L. *et al. Applied Geochemistry*, 2012, 27, (9), 1767–1782.

Gas hazard was evaluated in the three most important cold gas emission zones on the flanks of the quiescent Colli Albani volcano. These zones are located above structural highs of the buried carbonate basement that represents the main regional aquifer and the main reservoir for gas rising from depth. All extensional faults affecting the limestone reservoir represent leaking pathways along which gas rises to the surface and locally accumulates in shallow permeable horizons forming pressurized pockets that may produce gas blowout when reached by wells. The gas, mainly composed of CO_2 (>90 vol.%), contains appreciable quantities of H_2S (0.35–6 vol.%), and both represent a potentially high local hazard. Both gases are denser than air and accumulate near ground where they may reach hazardous concentrations, and lethal accidents frequently occur to animals watering at local ponds. In order to evaluate the rate of degassing and the related hazard, CO_2 and H_2S diffuse soil flux surveys have been repeatedly carried out using an accumulation chamber. The viscous gas flux of some important discrete emissions has been evaluated and the CO_2 and H_2S air concentration measured by portable devices and by tuneable diode laser profiles. The minimum potential lethal concentration of the two gases (250 ppm for H_2S and 8 vol.% for CO_2) is 320 times higher for CO_2, whereas the CO_2/H_2S concentration ratio in the emitted natural gas is significantly lower (15–159). This explains why H_2S reaches hazardous, even lethal, concentrations more frequently than CO_2. A relevant hazard exists for both gases in the depressed zones (channels, excavations) particularly in the non-windy early hours of the day.

13/01240 Housing managers key to reducing the greenhouse gas emissions of multi-family housing companies? A mixed method approach

Kyrö, R. *et al. Building and Environment*, 2012, 56, 203–210.

The building industry is facing a huge challenge as the industry sector carries much responsibility of the anthropogenic climate change: activities associated with housing alone account for as much as 30% of global annual energy demand. This demand derives not only from the physical characteristics of the buildings, but from the actions of the users, both end-users and professional managers. Even the best designed low-energy buildings will not perform as planned, if they are not operated properly. This study focuses on the role of professional managers in the energy and greenhouse gas (GHG) performance of existing urban and suburban housing. Several different types of housing companies with different housing managers are studied by both quantitative (input–output based hybrid life cycle analysis to estimate building performance) and qualitative (interviews to determine manager awareness and attitudes) means. It can be inferred from the study that housing managers through their attitudes and practices have a significant impact on the energy performance of buildings. Notwithstanding, managers feel as though they do not either have the responsibility or the power to make energy conservation a priority. Financial (long payback time) and even social (occupant discomfort) arguments are used to justify the lack of action. While housing managers readily hold the data, and have the professional skills for effective energy management, managers appear not to have an ethical motive for practicing energy-efficiency. In other words, managers have the potential to reduce the GHG emissions of housing companies, but the potential is currently not fully exploited.

13/01241 Intensification of NO_x absorption process by means of ozone injection into exhaust gas stream

Skalska, K. *et al. Chemical Engineering and Processing: Process Intensification*, 2012, 61, 69–74.

The growing emissions of nitrogen oxides into atmosphere endanger the human health and degrade the environment. In this work the application of ozone for the oxidation of nitrogen oxides present in exhaust gases was described. The main concept of the process is to oxidize nitrogen monoxide (NO) and nitrogen dioxide (NO_2) into dinitrogen pentoxide (N_2O_5) which reacts with water giving nitric acid. This way nitrogen oxides (NO_x) can be absorbed in water with good effectiveness. This study investigated the influence of the NO initial concentration and the ratio of NO/NO_2 in reaction gases on the NO conversion and selectivities into products. Furthermore, the two stage process composed of NO_x ozonation and the subsequent absorption of reaction gases in the 0.01 M solution of NaOH was performed. This experiments proved that due to ozonation the efficiency of NO_x absorption process is much higher than without ozone injection.

13/01242 Mechanism and prediction analysis of sustained casing pressure in 'A' annulus of CO_2 injection well

Zhu, H. *et al. Journal of Petroleum Science and Engineering*, 2012, 92–93, 1–10.

High value of sustained casing pressure (SCP) threatens the wellbore essential safety and environmental protection seriously. Considering the special and complex characteristic of SCP in 'A' annulus of CO_2 injection well, a prediction model of build-up of casing pressure has been proposed in this paper. Then finite difference method was used to solve the discrete equations in order to predict the SCP variation with time. The value is closely related to size and position of leak point, leakage rate, height of annular protective liquid, length of gas column at wellhead and the state of CO_2. The build-up of SCP in one well in the Jilin Oilfield is obtained by this model, which is in good agreement with the actual result, verifying the reliability of coupled model and calculation method.

13/01243 Microkinetic modeling of lean NO_x trap chemistry

Larson, R. S. *et al. Chemical Engineering Journal*, 2012, 189–190, 134–147.

A microkinetic chemical reaction mechanism capable of describing both the storage and regeneration processes in a fully formulated lean NO_x trap is presented. The mechanism includes steps occurring on the precious metal, NO_x storage, and oxygen storage sites of the catalyst. The complete reaction set is used with a transient plug flow reactor code (including boundary layer mass transfer) to simulate not only storage/regeneration cycles with a CO/H_2 reductant, but also steady flow temperature sweep experiments that were previously analysed with just a precious metal mechanism and a simpler steady state code. The results imply that NO_x storage was not negligible during some of the temperature ramps, necessitating a re-evaluation of the precious metal kinetic parameters. The parameters for the entire mechanism are inferred by finding the best overall fit to the complete set of experiments. Rigorous thermodynamic consistency is enforced for parallel reaction pathways and with respect to known data for all gas phase species. It is found that nearly all of the basic experimental observations can be reproduced with the transient simulations.

13/01244 Modeling of CBM production, CO_2 injection, and tracer movement at a field CO_2 sequestration site

Siriwardane, H. J. *et al. International Journal of Coal Geology*, 2012, 96–97, 120–136.

Sequestration of carbon dioxide in unmineable coal seams is a potential technology mainly because of the potential for simultaneous enhanced coalbed methane production (ECBM). Several pilot tests have been performed around the globe leading to mixed results. Numerous modelling efforts have been carried out successfully to model methane production and carbon dioxide (CO_2) injection. Sensitivity analyses and history matching along with several optimization tools were used to estimate reservoir properties and to investigate reservoir performance. Geological and geophysical techniques have also been used to characterize field sequestration sites and to inspect reservoir heterogeneity. The fate and movement of injected CO_2 can be determined by using several monitoring techniques. Monitoring of perfluorocarbon (PFC) tracers is one of these monitoring technologies. As a part of this monitoring technique, a small fraction of a traceable fluid is added to the injection wellhead along with the CO_2 stream at different times to monitor the timing and location of the breakthrough in nearby monitoring wells or offset production wells. A reservoir modelling study was performed to simulate a pilot sequestration site located in the San Juan coal basin of northern New Mexico. Several unknown reservoir properties at the field site were estimated by modelling the coal seam as a dual porosity formation and by history matching the methane production and CO_2 injection. In addition to reservoir modelling of methane production and CO_2 injection, tracer injection was modelled. Tracers serve as a surrogate for determining potential leakage of CO_2. The tracer was modelled as a non-reactive gas and was injected into the reservoir as a mixture along with CO_2. Geologic and geometric details of the field site, numerical modelling details of methane production, CO_2 injection, and tracer injection are presented in this paper. Moreover, the numerical predictions of the tracer arrival times were compared with the measured field data. Results show that tracer modelling is useful in investigating movement of injected CO_2 into the coal seam at the field site. Also, such new modelling techniques can be utilized to determine potential leakage pathways, and to investigate reservoir anisotropy and heterogeneity.

13/01245 New thermal-reactive reservoir engineering model predicts hydrogen sulfide generation in steam assisted gravity drainage

Kapadia, P. R. *et al. Journal of Petroleum Science and Engineering*, 2012, 94–95, 100–111.

In steam-assisted gravity drainage (SAGD), high-pressure, high-temperature steam is injected into a bitumen-bearing oil sands formation. For most operations, the steam temperature ranges from about 200 to 260 °C and thus under these conditions, the bitumen undergoes hydrous pyrolysis, i.e. aquathermolysis, yielding acid gases such as hydrogen sulfide and carbon dioxide. Current SAGD thermal reservoir simulation models often take into account complex spatial heterogeneity of the geology and oil composition and the physics of heat transfer, multiphase flow, gas solubility effects, and viscosity variations with temperature, however, none so far in the literature take the detailed chemistry and reaction engineering of bitumen aquathermolysis during field scale SAGD into account. Here, aquathermolysis reactions were added to a thermal reservoir simulation model to understand the reactive zones in the SAGD process and how the process generates acid gases via aquathermolysis. The results reveal that chemical reactions have a significant effect on the growth of the SAGD steam chamber and that the majority of the reactive zone is in the liquid pool that sits above the production well. The product gases of aquathermolysis reduce the efficiency of steam heat delivery capacity to the chamber edge. The results demonstrate that this effect can be reduced by lowering the steam injection pressure. This new model is capable of predicting acid gases like hydrogen sulfide, carbon oxides and fuel gases like hydrogen, methane as observed during SAGD field operations.

13/01246 Optimum liquefaction fraction for boil-off gas reliquefaction system of semi-pressurized liquid CO_2 carriers based on economic evaluation

Chu, B. *et al. International Journal of Greenhouse Gas Control*, 2012, 10, 46–55.

This investigation studied the optimum reliquefaction fraction of a boil-off gas reliquefaction system for semi-pressurized liquid CO_2 carriers. To prevent the overpressure of cargo tanks, the boil-off gas should be properly treated in suitable ways: to be vented into the atmosphere or to be liquefied in a dedicated liquefaction system. Because the former accompanies the penalty of carbon tax and the latter requires energy consumption, there is an optimum reliquefaction fraction minimizing the total treatment expense. To estimate the optimum reliquefaction fraction, the total treatment expense was composed of the three terms: the reliquefaction expense, the emission penalty, and the benefit of CO_2 sale, which were expressed by the reliquefaction fraction and other variables. The reliquefaction expense increased rapidly with the reliquefaction fraction, while the other two showed a linear dependence. Even though each term of the total treatment expense varied with the crude price, the CO_2 sale price, and the carbon tax, the optimum reliquefaction fraction was found to stay within a narrow region, roughly between 95.7% and 98.2% for all the plausible scenarios for the variables.

13/01247 Properties of activated cokes used for flue gas treatment in industrial waste incineration plants

Jastrząb, K. *Fuel Processing Technology*, 2012, 101, 16–22.

Properties of three types of AKP granular activated cokes (Gryfskand/Poland) used for flue gas treatment in industrial waste incineration plants were analysed. As a reference material activated coke FAK-5 (CarboTech/Germany) was used, commonly applied in BF technologies. Mechanical and physicochemical properties of the analysed materials, as well as their porous structure were determined. It was proven that intensive activation contributed to the increase of specific surface area from 218 to 386 m^2/g and greater volume of micropores. Moreover, significant weakening of mechanical properties and increased chemical use of carbon material were observed. Methodology for testing adsorptive capacity of SO_2 and Hg, and catalytic activity of NO reduction – under conditions similar to industrial ones – was developed. It was shown that the adsorptive activity of activated cokes for SO_2 and Hg was a linear function of a specific surface area. Catalytic properties with relation to nitric oxides depend on the content of ash and elementary carbon. It was proven that the intensity of activation should be a compromise between good sorptive properties and appropriate mechanical and catalytic properties.

13/01248 The effects of operating conditions on particulate matter exhaust from diesel locomotive engines

Park, D. *et al. Science of the Total Environment*, 2012, 419, 76–80.

Numerous reports have shown that fine particulates threaten human health. Since their health impact is associated with both mass and number concentrations, it is necessary to evaluate the emission standards for particulate mass accordingly. This study examined the particulate matter characteristics of diesel locomotive engine exhaust at various engine ratings. Diesel engine exhaust was collected via a dilution tunnel and the concentration and size distribution of fine particles were measured by a scanning mobility particle sizer. Exhaust gasses were measured simultaneously by a stack sampler. The maximum carbon monoxide emission was reached at 59% of the maximum rating, after which emissions decreased. The particle count median diameter increased with the engine rating, until a maximum was reached at 40% of the maximum rating. Most exhaust particles were nanoparticles with the nuclei mode range, a particle diameter (D_P) < 50 nm. The increase in particles with the accumulation mode range, $50 < D_P < 1000$ nm, led to a mass concentration increase and number concentration reduction. The count median diameter was within the nuclei mode range at lower engine ratings, and within the accumulation mode range at higher engine ratings. Since diesel engines mainly generate fine particles, exhaust particle mass and size distribution should be considered in emission regulations.

Hydrocarbon emissions

13/01249 Environmental strategies to remove volatile aromatic fractions (BTEX) from petroleum industry wastewater using biomass

Costa, A. S. *et al. Bioresource Technology*, 2012, 105, 31–39.

This work investigates the potentials of peat and angico hardwood sawdust to remove BTEX (benzene, toluene, ethylbenzene, and isomers of xylene) from the produced water discharged into aquatic systems during petroleum extraction. Peat and angico sawdust samples were pyrolysed at 500 °C, and found to contain *n*-alkenes, *n*-alkanes and pentacyclic triterpenes (peat), and 4-methoxyphenol, 1,4-dimethoxyphenol and 1,3,4-trimethoxyphenol (angico sawdust). In batch experiments, the removal capacities using peat were 32.4%, 50.0%, 63.0%, 67.8% and 61.8% for benzene, toluene, ethylbenzene, *m,p*-xylenes and *o*-xylene, respectively. This compared with removal capacities using angico sawdust of 20.2%, 36.4%, 52.8%, 57.8% and 53.7% for these compounds respectively, demonstrating the superior performance of the peat.

13/01250 Modeling spiral-wound membrane modules with applications for gas/vapor permeation

Lin, D. *et al. Computers & Chemical Engineering*, 2012, 44, 20–33.

Gas/vapour permeation has become a common method for volatile organic compound recovery and CO_2 capture. The spiral-wound membrane module, which has high packing density, has been commonly used in gas/vapour permeation. In this study, the model that suits the spiral-wound polydimethylsiloxane membrane is obtained by using an integral transform from a Navier–Stokes equation and a mass transfer differential equation. The predicted results indicate that the concentration polarization and spiral-wound membrane structure influence can be neglected. The mass transfer based on the MS–UNIQUAC (MS–U) model is also proposed and compared to that based on the Fick–Henry (F–H) model. The comparison results show that the mass transfer based on the F–H model can only be used in a gas mixture without condensable gas; the MS–U model should be used for a gas mixture that includes condensable gas. The influence of permeate flux and feed-side composition in the spiral-wound membrane at different operation conditions is also investigated using the MS–U model.

13/01251 Modified Fenton oxidation of polycyclic aromatic hydrocarbon (PAH)-contaminated soils and the potential of bioremediation as post-treatment

Venny, S. G. *et al. Science of the Total Environment*, 2012, 419, 240–249.

This work focuses on the remediation of polycyclic aromatic hydrocarbon (PAH)-contaminated soil using modified Fenton (MF) treatment coupled with a novel chelating agent (CA), a more effective technique among currently available technologies. The performance of MF treatment to promote PAH oxidation in artificially contaminated soil was investigated in a packed column with a hydrogen peroxide (H_2O_2) delivery system simulating *in situ* soil flushing which is more representative of field conditions. The effectiveness of process parameters H_2O_2/soil, Fe^{3+}/soil, CA/soil weight ratios and reaction time were studied using a 2^4 three level factorial design experiments. An optimized operating condition of the MF treatment was observed at H_2O_2/soil 0.05, Fe^{3+}/soil 0.025, CA/soil 0.04 and 3 h reaction time with 79.42% and 68.08% PAH removals attainable for the upper and lower parts of the soil column respectively. The effects of natural attenuation and biostimulation process as post-treatment in the remediation of the PAH-contaminated soil were also studied. In all cases, three-aromatic ring PAH (phenanthrene) was more readily degraded than four-aromatic ring PAH (fluoranthene) regardless of the bioremediation approach. The results revealed that both natural attenuation and biostimulation could offer remarkable enhancement of up to 6.34% and 9.38% in PAH removals respectively after 8 weeks of incubation period. Overall, the results demonstrated that combined inorganic CA-enhanced MF treatment and bioremediation serves as a suitable strategy to enhance soil quality particularly to remediate soils heavily contaminated with mixtures of PAHs.

Life cycle analysis

13/01252 A comparative life cycle analysis of low power PV lighting products for rural areas in South East Asia

Durlinger, B. *et al. Renewable Energy*, 2012, 41, 96–104.

This paper evaluates the environmental effects of low-power photovoltaic (PV) lighting products, which are increasingly used in rural areas in South-east Asia, by means of a life cycle analysis (LCA). The main goals of the project are to determine (1) the environmental impacts, (2) which parts are contributing to environmental impacts that occur, and (3) the accuracy of an LCA of these PV products. The study is based on an entrepreneurial case in Cambodia. Three PV lighting products with a nominal power of 0.7, 4.5 and 40 Wp, respectively, have been compared with three alternatives for lighting services. The LCA was executed with Simapro software using the Ecoinvent 2.1 database and applying the ReCiPe 2008 method for the impact assessment. An important conclusion of the study is that solar PV lighting products have less environmental impact than conventional lighting solutions, such as lighting services from kerosene lamps and compact fluorescent lamps powered by car batteries. The environmental profile of small size PV lighting products can be improved by approximately 50% by recycling of the batteries. From an evaluation of the accuracy of an LCA of PV lighting products, it can be concluded that impacts of these PV lighting products are lower or comparable to those of lighting by compact fluorescent lights powered by electricity from the grid in the South-east Asian context. As such, they offer an environmentally beneficial lighting service for off-grid households.

13/01253 A methodology to estimate greenhouse gases emissions in life cycle inventories of wastewater treatment plants

Rodriguez-Garcia, G. *et al. Environmental Impact Assessment Review*, 2012, 37, 37–46.

The main objective of this paper is to present the direct emissions estimation model (DEEM), a model for the estimation of CO_2 and N_2O emissions from a wastewater treatment plant (WWTP). This model is consistent with non-specific but widely used models such as AS/AD and ASM #1 and presents the benefits of simplicity and application over a common WWTP simulation platform, BioWin®, making it suitable for life cycle assessment and carbon footprint studies. Its application in a Spanish WWTP indicates direct N_2O emissions to be eight times larger than those associated with electricity use and thus relevant for LCA. CO_2 emissions can be of similar importance to electricity-associated ones provided that 20% of them are of non-biogenic origin.

13/01254 Climate impacts of bioenergy: inclusion of carbon cycle and albedo dynamics in life cycle impact assessment

Bright, R. M. *et al. Environmental Impact Assessment Review*, 2012, 37, 2–11.

Life cycle assessment (LCA) can be an invaluable tool for the structured environmental impact assessment of bioenergy product systems. However, the methodology's static temporal and spatial scope combined with its restriction to emission-based metrics in life cycle impact assessment (LCIA) inhibits its effectiveness at assessing climate change impacts that stem from dynamic land surface–atmosphere interactions inherent to all biomass-based product systems. This paper focuses on two dynamic issues related to anthropogenic land use that can significantly influence the climate impacts of bioenergy systems – (i) temporary changes to the terrestrial carbon cycle and (ii) temporary changes in land surface albedo – and illustrates how they can be integrated within the LCA framework. In the context of active land use management for bioenergy, the authors discuss these dynamics and their relevancy and outline the methodological steps that would be required to derive case-specific biogenic CO_2 and albedo change characterization factors for inclusion in LCIA. They demonstrate their concepts and metrics with application to a case study of transportation biofuel sourced from managed boreal forest biomass in northern Europe. GWP indices are derived for three land management cases of varying site productivities to illustrate the importance and need to consider case- or region-specific characterization factors for bioenergy product systems. Uncertainties and limitations of the proposed metrics are discussed.

13/01255 Comparative life cycle assessment of hydrogen and other selected fuels

Hacatoglu, K. *et al. International Journal of Hydrogen Energy*, 2012, 37, (13), 9933–9940.

A streamlined life cycle assessment (LCA) is reported of a nuclear-based copper–chlorine (Cu–Cl) hydrogen production cycle, including estimates of fossil fuel energy use and greenhouse gas (GHG) emissions. Calculations revealed that the process requires 474 kJ of fossil fuel energy per MJ of hydrogen, which is less than for other hydrogen production processes. Moreover, GHG emissions are estimated to be 27 gCO_2e per MJ of hydrogen, which is only slightly higher than the corresponding value for wind-based hydrogen production. A sensitivity analysis demonstrated that the performance of the system could be further improved at higher yields of hydrogen. Although the system significantly outperformed fossil-based gasoline and hydrogen production pathways, the integrated nuclear and thermochemical cycle still requires significant research and development before commercialization is possible.

13/01256 Impact of energy supply infrastructure in life cycle analysis of hydrogen and electric systems applied to the Portuguese transportation sector

Lucas, A. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 10973–10985.

Hydrogen and electric vehicle technologies are being considered as possible solutions to mitigate environmental burdens and fossil fuel dependency. Life cycle analysis (LCA) of energy use and emissions has been used with alternative vehicle technologies to assess the well-to-wheel (WTW) fuel cycle or the cradle-to-grave (CTG) cycle of a vehicle's materials. Fuel infrastructures, however, have thus far been neglected. This study presents an approach to evaluate energy use and CO_2 emissions associated with the construction, maintenance and decommissioning of energy supply infrastructures using the Portuguese transportation system as a case study. Five light-duty vehicle technologies are considered: conventional gasoline and diesel (ICE), pure electric (EV), fuel cell hybrid (FCHEV) and fuel cell plug-in hybrid (FC-PHEV). With regard to hydrogen supply, two pathways are analysed: centralized steam methane reforming (SMR) and on-site electrolysis conversion. Fast, normal and home options are considered for electric chargers. The authors conclude that energy supply infrastructures for FC vehicles are the most intensive with 0.03–0.53 MJ_{eq}/MJ emitting 0.7–27.3 g CO_{2eq}/MJ of final fuel. While fossil fuel infrastructures may be considered negligible (presenting values below 2.5%), alternative technologies are not negligible when their overall LCA contribution is considered. EV and FCHEV using electrolysis report the highest infrastructure impact from emissions with approximately 8.4% and 8.3%, respectively. Overall contributions including uncertainty do not go beyond 12%.

13/01257 LCA of cropping systems with different external input levels for energetic purposes

Goglio, P. *et al. Biomass and Bioenergy*, 2012, 42, 33–42.

Biofuels could become increasingly important for agriculture; however there is growing concern regarding the possible environmental drawbacks due to the risks of increased inputs during crop cultivation. These risks need to be evaluated in order to assess the best management practices. In this study, a life cycle assessment (LCA) was carried out: (i) to evaluate the environmental impacts of three cropping systems characterized by different external input levels (low S1, medium S2 and high S3) applied to sunflower and maize, both in rotation with wheat, in a Mediterranean region; (ii) to estimate the environmental benefits of the optimization of cropping systems for energy management. Output–input ratio, net energy balance, global warming potential (GWP), eutrophication potential (EP) and acidification potential (AP) were used as LCA impact categories. Data from cropping systems (external input and crop yields) were collected from a long-term experiment carried out in the coastal plain of Tuscany; data regarding fertilizers, machinery and pesticide production were taken from literature. The results obtained showed S1 with the highest output–input ratios and the lowest impact for the selected impact categories. The other cropping systems S2 and S3 showed limited differences between them for all the impact categories evaluated. Fertilizer use and application, irrigation and machinery use caused most of the environmental impacts and energy consumption. The allocation procedure, showing residues as co-products, had a strong influence on the overall efficiency of agricultural systems.

13/01258 Life cycle assessment applied to electricity generation from renewable biomass

Perilhon, C. *et al. Energy Procedia*, 2012, 18, 165–176.

This work concerns the production of electricity from renewable sources produced from biomass (wood waste) in cogeneration plants. Two facilities are compared: a 2 MW electricity power plant and a 10 MW one. They are also compared to electricity production in a diesel engine cogeneration. The objective is to compare the environmental impact of various power plants, using two different fuels and/or of different power. A detailed life cycle assessment methodology is therefore presented. The results – in favour of the 2 MW wood plant but sensitive to assumptions – are then discussed.

13/01259 Life cycle assessment of municipal solid waste treatment to energy options: case study of KARTAMANTUL region, Yogyakarta

Gunamantha, M. and Sarto, *Renewable Energy*, 2012, 41, 277–284.

Various methods of solid waste treatment are available. However, due to heterogeneity characteristic of solid waste, determined the best means to manage solid waste in environmental view of point is not straightforward. In this case, solid waste management scenarios and an environmental analysis tool are required. This study compared various energetic valorization options with each other using the simplified life cycle assessment methodology. These scenarios were landfilling without energy recovery as a representative of existing solid waste management, landfilling with energy recovery, combination of incineration and anaerobic digestion, combination of gasification and anaerobic digestion, direct incineration, and direct gasification. A case study area in a typical KARTAMANTUL (acronym of three cities: Yogyakarta, Sleman, Bantul) intercity region in province of Yogyakarta, Indonesia. One ton of solid waste treated was defined as the functional unit of the systems studied. The life cycle inventory analysis was done by including field and laboratory survey to characterize solid waste in area study and using emission factors which were adopted from literature to estimate environmental burdens for each scenario. Inventory's result was classified into impact categories, i.e. global warming, acidification, eutrophication, and photochemical oxidant formation. The indicators of categories were quantified by using the equivalence factors of relevant emissions to determine the environmental performance of each scenario. The study shown that in most of the impact categories (except acidification), a scenario with direct gasification indicated the best environmental profile. A sensitivity analysis was also conducted to examine change in outcomes for a variety of organic biowaste inputs, but had no significant effect on the overall result.

13/01260 Life cycle energy and greenhouse gas profile of a process for the production of ammonium sulfate from nitrogen-fixing photosynthetic cyanobacteria

Razon, L. F. *Bioresource Technology*, 2012, 107, 339–346.

In this paper, an alternative means for nitrogen fixation that may consume less energy and release less greenhouse gases than the Haber–Bosch process is explored. A life-cycle assessment was conducted on a process to: culture the cyanobacterium, *Anabaena* sp. ATCC 33047, in open ponds; harvest the biomass and exopolysaccharides and convert these to biogas; strip and convert the ammonia from the biogas residue to ammonium sulfate; dry the ammonium sulfate solution to ammonium sulfate crystals and transport the finished product. The results suggest that substantial reductions in non-renewable energy use and greenhouse gas emissions may be realized. The study opens the possibility that Haber–Bosch ammonia may be replaced with ammonia from a biomass process which simultaneously generates renewable energy. The process is intrinsically safer than the Haber–Bosch process. However, there are trade-offs in terms of land use and possibly, water.

13/01261 Life-cycle assessment of a house with alternative exterior walls: comparison of three impact assessment methods

Monteiro, H. and Freire, F. *Energy and Buildings*, 2012, 47, 572–583.

A life-cycle (LC) model has been implemented for a Portuguese single-family house. The first goal is to characterize the main LC processes (material production and transport, heating, cooling, maintenance) assessing seven alternative exterior walls for the same house to identify environmentally preferable solutions. The second goal is to compare the results of three life-cycle impact assessment (LCIA) methods – CED (cumulative energy demand), for primary energy accounting; CML 2001 (Institute of Environmental Sciences of Leiden University) and EI'99 (Eco-indicator'99), for multiple environmental impacts – to determine the extent to which the results of a life-cycle assessment are influenced by the method applied. The results show that the most significant LC process depends on the operational pattern assumed. Regarding the assessment of the exterior wall alternatives, the results indicate the wood-wall is the preferable solution. Non-renewable CED shows results similar to abiotic depletion (CML 2001) and resources (EI'99) categories, as well as some correlation with climate change/global warming potential (GWP), acidification and eutrophication. However, no correlation was found with the remaining impact categories. Comparing CML 2001 and EI'99 categories, GWP, ozone layer depletion, abiotic depletion, acidification, and eutrophication present robust results that permit a straightforward comparison between the two LCIA methods. Nevertheless, CML results present slightly higher impacts for the use phase, while EI'99 for material production. In addition, the two LCIA methods can present inconsistent results between similar categories (different ranking of alternatives), which ultimately can influence the choice among solutions.

13/01262 Production of enriched methane by a molten-salt concentrated solar power plant coupled with a steam reforming process: an LCA study

Piemonte, V. *et al. International Journal of Hydrogen Energy*, 2012, 37, (15), 11556–11561.

Enriched methane (EM) is a gas mixture consisting of methane and a certain amount of hydrogen (10–30%vol) that finds out several applications such as fuel of internal combustion engines (ICEs). To produce EM, a steam reforming reactor whose heat duty is supplied by a molten-salt stream heated up by a concentrating solar power (CSP) plant can be used, in order to generate the hydrogen steam by solar energy. In fact, molten salts at temperatures up to 550 °C can allow to reach the necessary thermal level inside the reactor to promote steam reforming reaction. The combination of technologies such as EM steam reformer, concentrating solar power (CSP) systems and molten-salt heat carriers, allows a partial decarbonation of the fossil fuel, thanks to the production of hydrogen, together with the possibility to carry solar energy in the current natural gas grid. The aim of this work is to present a life cycle assessment of a novel hybrid plant for the production of EM from a solar steam reforming reactor. The performance, of this innovative architecture have been evaluated from an environmental point of view by the use of a life cycle analysis software (SimaPro7) and compared with the ones of traditional plants (reformer and cracker for the hydrogen production). The results highlight the lower environmental footprint of this innovative plant compared to the environmental impact of the two traditional plant considered in this work. The fossil energy duty of the MS-CSP-SR plant is about 50% less than that required from the conventional cracker and reformer production plants. The conventional plants are also characterized by a global warming potential of about 75% higher than that of the MS-CSP-SR plant.

13/01263 Reduction of environmental and energy footprint of microalgal biodiesel production through material and energy integration

Chowdhury, R. *et al. Bioresource Technology*, 2012, 108, 102–111.

The life cycle impacts were assessed for an integrated microalgal biodiesel production system that facilitates energy- and nutrient-recovery through anaerobic digestion, and utilizes glycerol generated within the facility for additional heterotrophic biodiesel production. Results show that when external fossil energy inputs are lowered through process integration, the energy demand, global warming potential (GWP), and process water demand decrease significantly and become less sensitive to algal lipid content. When substitution allocation is used to assign additional credit for avoidance of fossil energy use (through utilization of recycled nutrients and biogas), GWP and water demand can, in fact, increase with increase in lipid content. Relative to stand-alone algal biofuel facilities, energy demand can be lowered by 3–14 GJ per ton of biodiesel through process integration. GWP of biodiesel from the integrated system can be lowered by up to 71% compared to petroleum fuel. Evaporative water loss was the primary water demand driver.

13/01264 The technology life cycle: conceptualization and managerial implications

Taylor, M. and Taylor, A. *International Journal of Production Economics*, 2012, 140, (1), 541–553.

This paper argues that the technology life cycle literature is confused and incomplete. This literature is first reviewed with consideration of the related concepts of the life cycles for industries and products. By exploring the inter-relationships between these, an integrated view of the technology life cycle is produced. A new conceptualization of the technology life cycle is then proposed. This is represented as a model that incorporates three different levels for technology application, paradigm and generation. The model shows how separate paradigms emerge over time to achieve a given application. It traces the eras of ferment and incremental change and shows how technology generations evolve within these. It also depicts how the eras are separated by the emergence of a dominant design, and how paradigms are replaced at a technological discontinuity. By adopting this structure, the model can demarcate the evolution of technologies at varying levels of granularity from the specific products in which they may be manifest to the industries in which they are exploited. By taking technology as the unit of analysis the model departs from previous work, which has adopted a product-based perspective predominantly. The paper discusses the managerial and research implications associated with the technology life cycle, and indicates how these inform future research directions. As well as contributing to academic knowledge, the results of this research are of value to those who make decisions about the development, exploitation and use of technology including technology developers, engineers, technologists, R&D managers, and designers.

16 ENERGY

Supplies, policy, economics, forecasts

13/01265 A comprehensive approach to the design of ethanol supply chains including carbon trading effects

Giarola, S. *et al. Bioresource Technology*, 2012, 107, 175–185.

The optimal design of biofuels production systems is a key component in the analysis of the environmental and economic performance of new sustainable transport systems. In this paper a general mixed integer linear programming modelling framework is developed to assess the design and planning of a multi-period and multi-echelon bioethanol upstream supply chain under market uncertainty. The optimization design process of biofuels production systems aims at selecting the best biomass and technologies options among several alternatives according to economic and environmental (global warming potential) performance. A key feature in the proposed approach is the acknowledgement of an economic value to the overall greenhouse gas emissions, which is implemented through an emissions allowances trading scheme. The future Italian biomass-based ethanol production is adopted as a case study. Results show the effectiveness of the model as a decision-making tool to steer long-term decisions and investments.

13/01266 A method to compare simulated and measured data to assess building energy performance

Maile, T. *et al. Building and Environment*, 2012, 56, 241–251.

Building energy performance is often inadequate given design goals. While different types of assessment methods exist, they either do not consider design goals and/or are not general enough to integrate new and innovative energy concepts. Furthermore, existing assessment methods focus mostly on the building and system level while ignoring more detailed data. With the availability and affordability of more detailed measured data, the increased number of measured data points requires a structure to organize these data. This paper presents the energy performance comparison methodology (EPCM), which enables the identification of performance problems based on a comparison of measured data and simulated data representing design goals. The EPCM is based on an interlinked building object hierarchy that structures the detailed performance data from a spatial and mechanical perspective. This research is developed and tested on multiple case studies that provide real-life context and more generality compared to single case studies.

13/01267 Accounting for forest carbon pool dynamics in product carbon footprints: challenges and opportunities

Newell, J. P. and Vos, R. O. *Environmental Impact Assessment Review*, 2012, 37, 23–36.

Modification and loss of forests due to natural and anthropogenic disturbance contribute an estimated 20% of annual greenhouse gas (GHG) emissions worldwide. Although forest carbon pool modelling rarely suggests a ‘carbon neutral’ flux profile, the life cycle assessment community and associated product carbon footprint protocols have struggled to account for the GHG emissions associated with forestry, specifically, and land use generally. Principally, this is due to underdeveloped linkages between life cycle inventory (LCI) modelling for wood and forest carbon modelling for a full range of forest types and harvest practices, as well as a lack of transparency in globalized forest supply chains. In this paper, through a comparative study of US- and Chinese-coated freesheet paper, the initial foundations for a methodology were developed that rescales IPCC methods from the national to the product level, with reference to the approaches in three international product carbon footprint protocols. Due to differences in geographic origin of the wood fibre, the results for two scenarios are highly divergent. This suggests that both wood LCI models and the protocols need further development to capture the range of spatial and temporal dimensions for supply chains (and the associated land use change and modification) for specific product systems. The paper concludes by outlining opportunities to measure and reduce uncertainty in accounting for net emissions of biogenic carbon from forestland, where timber is harvested for consumer products.

13/01268 Development and analysis of climate sensitivity and climate adaptation opportunities indices for buildings

Pyke, C. R. *et al. Building and Environment*, 2012, 55, 141–149.

Buildings represent long-term, capital-intensive investments designed to perform for decades into the future. Consequently, the potential for changes in climate across the design lifetime of built environments represents an immediate challenge for planning, design, and construction. This study considered the opportunities to assess climate sensitivity and adaptive opportunities associated with green building practice. This developed a pair of complementary indicators called the ‘climate sensitivity index’ (CSI) and the ‘climate adaptation opportunity index’ (CAOI). These indicators are applied to evaluate individual strategies (‘credits’) within the ‘Leadership in Energy and Environmental Design’ (LEED$^{\text{TM}}$) for new construction rating system. The indices provide two complementary scores for each strategy. The CSI reflects potential sensitivity to changing conditions (i.e. risks to performance outcomes), and the CAOI indicates potential adaptive opportunities (i.e. plausible strategies to adapt to changing conditions). The authors apply the indices to retrospectively examine the prevalence of potentially sensitive and adaptive practices among a global set of 2440 LEED-certified projects. Adaptive opportunities were more prevalent than sensitivities in the LEED-NC rating system. The CSI and CAOI indices illustrate how information can be derived by interpreting patterns of LEED credit achievement. The indices will be available within a suite of analytical tools in the green building information gateway.

13/01269 Energy policy in the context of sustainable development: case of Algeria and Tunisia

Ghezloun, A. *et al. Energy Procedia*, 2012, 18, 53–60.

A study of the Algerian National Agency for Energy Management (APRUE) indicates that energy demand will explode by 2020. The needs of the residential sector will be multiplied by 2.7 while the tertiary sector will increase its power consumption by 3.2, an increase of 40% relative to current consumption. In Algeria, despite a considerable potential, the share of renewable energies in the energy balance is still low especially in the production of electricity, is only 0.02% of national electricity consumption (5 GWh). The rise of renewable energies in Algeria cannot be conceived without the completion of a phased program more important of projects to produce electricity. Energy policy should encourage the introduction of hybrid possibilities and support other forms, including electricity generation by the private sector to share the heavy burden. Taking advantage of rising energy prices and the need to limit the independence of external energy, combined with the growing sensitivity in relation to environmental problems, renewable energies prove a necessity for the sustainable development of Tunisia.

13/01270 Energy use, indoor temperature and possible adaptation strategies for air-conditioned office buildings in face of global warming

Guan, L. *Building and Environment*, 2012, 55, 8–19.

This paper discusses and summarizes a recent systematic study on the implication of global warming on air-conditioned office buildings in Australia. Four areas are covered, including analysis of historical weather data, generation of future weather data for the impact study of global warming, projection of building performance under various global warming scenarios, and evaluation of various adaptation strategies under 2070 high global warming conditions. Overall, it is found that depending on the assumed future climate scenarios and the location considered, the increase of total building energy use for the sample Australian office building may range from 0.4 to 15.1%. When the increase of annual average outdoor temperature exceeds 2 °C, the risk of overheating will increase significantly. However, the potential overheating problem could be completely eliminated if internal load density is significantly reduced.

13/01271 Geothermal energy potential in the St-Lawrence River area, Québec

Majorowicz, J. and Minea, V. *Geothermics*, 2012, 43, 25–36.

Previous estimates of geothermal energy potential in Canada give an indication of available heat to be 'farmed' at depth with focus on Western Canadian Cordillera and Western Canadian Sedimentary basin as prime targets. This paper examines in more detail temperature–depth relationships near large population centres in Québec, in order to provide a first order assessment of enhanced geothermal systems (EGS) potential for electrical and heat generation. Results show areas with significant EGS potential in the St-Lawrence River valley related to high heat flow density and thermal blanketing of thick sedimentary cover. At >120 °C found to be a prospect for several areas in Québec (drilled to depths of over 4.5 km in Trois-Rivières area, near 4.5 km in the Eastern St-Lawrence River (Rimouski, Gaspé and Golf, including Anticosti Island) and just 4 km in Québec area) the potentially available geothermal power from EGS hydrothermal systems in deep sediments can be of significance.

13/01272 Is green and profitable sustainable? Assessing the trade-off between economic and environmental aspects

Figge, F. and Hahn, T. *International Journal of Production Economics*, 2012, 140, (1), 92–102.

Businesses are more and more confronted with demands to play an active role to reduce environmental burdens effectively and to help to achieve environmental sustainability. The authors question the suitability of the green business case and argue that corporate environmental strategies need to aim at the creation of environmental value alongside economic value rather than the creation of economic value through environmental management. Three shortcomings of the green business case limit its usefulness to develop suitable corporate sustainability strategies. The authors contrast the green business case with an opportunity cost based approach for assessing the environmental performance of firms. The argument is then applied to an integrated analysis of the financial, carbon and VOC-performance of 16 major car manufacturers worldwide to illustrate how companies respond to the twofold scarcity of economic capital and natural resources as well as the role of proactive technology choices in this context. This analysis shows how firms can go beyond the standard green business case that ultimately limits environmental strategies to increasing capital efficiency. The authors argue that by applying the well-established notion of opportunity costs to the assessment of environmental resources besides economic capital, companies can identify strategies that create economic and environmental value and help to maximize the contribution to sustainability rather than to economic capital efficiency alone.

13/01273 Modeling the transition towards a sustainable energy production in developing nations

Thiam, D.-R. *et al. Applied Energy*, 2012, 94, 98–108.

The paper investigates how renewable technologies could promote the transition towards a sustainable energy production in developing nations. Based on two different developing nations in terms of economic, technological and institutional structure: South Africa and Senegal, the authors implemented scenarios in a bottom-up PowerPlan model in order to analyse the transition toward a sustainable electric production. Two scenarios have been considered: a business-as-usual (BAU) and a hybrid renewable energy (HRE) scenario. In the BAU scenario it was assumed that the electricity demand is entirely satisfied by an increase of the investment in the current supply structure based on fossil-fuel energy source. Whereas in the HRE scenario, the authors assume 20% and 30% of the electricity supply being generated from renewable resources by 2020 and 2030, respectively. Focusing on wind and solar photovoltaic technologies, the results show the cost-competitiveness of renewable energy deployment in South Africa. In the case of Senegal, the results show that fossil-fuel resource remains the most competitive to generate electricity in the nation during the next coming years as long as environmental advantages of renewable resource are not considered. This research indicates that in the case of a centralized electricity supply option, both a scale effect and a learning improvement could eventually strengthen the competitiveness of renewable technology deployment in developing nations.

13/01274 Power curve tracking in the presence of a tip speed constraint

Bottasso, C. L. *et al. Renewable Energy*, 2012, 40, (1), 1–12.

This paper considers the problem of power regulation for a variable speed wind turbine in the presence of a blade tip speed constraint, for example to limit noise emissions. The main contribution of the paper is the formulation of a policy for the regulation of the machine in the transition region between the classical regions *II* and *III* that accommodates the tip speed constraint, and the derivation of associated wind schedules for the rotor speed, blade pitch and aerodynamic torque. To exemplify the possible use of such wind schedules in the design of control laws, model-based controllers are formulated in this paper that are capable of performing power curve tracking throughout all wind speeds, in contrast with commonly adopted approaches that use switching controllers to cover the various operating regimes of the machine. The proposed regulation policies and control laws are demonstrated in a high fidelity simulation environment for a representative 3 MW machine.

13/01275 Production planning for vehicle recycling factories in the EU legislative and global business environments

Simic, V. and Dimitrijevic, B. *Resources, Conservation and Recycling*, 2012, 60, 78–88.

End-of-life vehicles (ELVs) are a priority in the EU waste flow, and data show that as many as 6.34 million vehicles were processed in 2008. This paper focuses on the production process in a vehicle recycling factory. It presents a tactical production planning problem for vehicle recycling factories in the EU legislative and global business environments. The problem is formulated as a linear program, which provides optimal storage, processing and recovery, recycling and landfill disposal route decisions. The proposed model can not only help vehicle recycling factories improve their eco-efficiency and profitability but also answer many important questions. The present paper deals with questions regarding which costs should be set in EU member states for landfill disposal, combustion in municipal solid waste incinerators and processing in advanced thermal treatment plants so that the ELV Directive can have the most positive eco-effect on the vehicle recycling factory business. The cost increase for landfill disposal will not always reduce the quantity of disposed automobile shredder residue. The influence of the ELV Directive on the vehicle recycling factory business is analysed. Future quotas will not endanger their profitability. Comprehensive testing of the proposed model showed that the control of the recycling system efficiency should be done at the system level because it will in no way jeopardize the ELV directive objectives.

13/01276 Shipping or local production? CO_2 impact of a strategic decision: an automotive industry case study

Nieuwenhuis, P. *et al. International Journal of Production Economics*, 2012, 140, (1), 138–148.

For Asian manufacturers the trade-off between shipping from domestic plants and investing in transplant facilities is of particular importance. Korean vehicles indirectly account for significant amounts of greenhouse gases as they travel. Here, an established transport cost model is adapted to track CO_2 emissions along the built-up vehicle supply chain from the final assembly plant to a local distribution location, taking the cases of Hyundai and Kia, such that initial estimates of the environmental impact of both the Korea–US and the Korea–Europe automotive supply chains may be made. It is found that in both cases the local option, even using road-based distribution, leads to significantly lower emissions than seaborne sourcing direct from South Korea.

13/01277 Understanding the pitfalls of CCS cost estimates

Rubin, E. S. *International Journal of Greenhouse Gas Control*, 2012, 10, 181–190.

This paper reviews and compares the prevailing methods, metrics and assumptions underlying cost estimates for CO_2 capture and storage (CCS) technologies applied to fossil fuel power plants. This assessment reveals a number of significant differences and inconsistencies across different studies, not only in key technical, economic and financial assumptions related to the cost of a CCS project (such as differences in plant size, fuel type, capacity factor, and cost of capital) but also in the underlying methods and cost elements that are included (or excluded) in a particular study (such as the omission of certain 'owner's' costs or the cost of transport and storage). Such differences often are not apparent in the cost results that are reported publicly or in the technical literature. In other cases, measures that have very different meanings (such as the costs of CO_2 avoided, CO_2 captured and CO_2 abated) are all reported in similar units of 'dollars per ton CO_2'. As a consequence, there is likely to be some degree confusion, misunderstanding and possible misrepresentation of CCS costs. Given the widespread interest in the cost of CCS and the potential for lower-cost CO_2 capture technology, methods to improve the consistency and transparency of CCS cost estimates are needed.

13/01278 Using UK climate change projections to adapt existing English homes for a warming climate

Gupta, R. and Gregg, M. *Building and Environment*, 2012, 55, 20–42.

This paper uses probabilistic climate change data from the UK climate change projections of 2009 to define extreme climate change in order to model the effect of future temperature change, particularly summer overheating on the energy consumption of, and comfort in, existing English homes (located in Oxford). Climate change risk is then analysed as a factor of climate hazard, exposure and vulnerability. With the risk of overheating theoretically identified, the risk of overheating and the future change impact on space heating energy use is then virtually detailed for four English home types modelled using future weather years in a dynamic simulation modelling software (IES). A range of passive adaptation measures are then critically reviewed with regard to their effectiveness in minimizing the negative impacts of climate change and to identify the most effective measures in reducing or eliminating the negative impacts of climate change on comfort and energy consumption. In addition the adaptation options are grouped and tested as packages in order to identify the optimal solution for adaptive retrofitting of English homes. For all homes modelled, user-controlled shading proved to be the most effective adaptation. Increasing the surface albedo of the building fabric and exposure of thermal mass were also revealed to be effective although proving to be complicated and requiring detailed consideration of the optimal locations. Ultimately among the passive options tested, the research found that none could completely eliminate the risk of overheating in the homes, particularly by the 2080s.

Energy conservation

13/01279 A decision support system for consumption optimization in a naphtha reforming plant

Biscarri, F. *et al. Computers & Chemical Engineering*, 2012, 44, 1–10.

In a naphtha distillation process, the natural objective is to perform an entire process maximization of the production rate while meeting required product qualities by searching for an optimal operating condition by manipulating the operating variables. The objective of this paper includes performing an energy process optimization. Not only is an adequate production rate met with the required product qualities but the operating cost is also minimized through a data mining approach. The study of the influence of all process attributes in the defined energy efficient indicator allows the construction of a multivariate linear model to aid human experts in the recovery of energy losses. A canonical discriminant function carried out the data prediction step. The quality of the decision support system framework is illustrated by a case study considering a real database. Also, a commercial software supported by this mining framework is presented.

13/01280 Analysis of carbon impact using mix energy sources for industrial heating applications. An assessment of options to refit services in an existing building

Gil-López, T. *et al. Fuel Processing Technology*, 2012, 103, 151–159.

With respect to industrial buildings, this study aims to clarify what would be the most efficient way of heating, considering at the same time its economic viability. Therefore, the study presents an integrated approach to heating and ventilation system to identify the most adequate of them in the case of an existing workshop. The object of the study is a solar heating system, with three auxiliary power options: an oil fuel boiler combined with a flue gas condensing unit, an electric boiler and a condensing gas boiler. The heating system is designed so that the primary energy only comes in on line when the solar energy contribution is not sufficient. The results of the study, from the point of economic viability as well as of energy efficiency and impact on carbon footprint, show that the natural gas condensing boilers with solar thermal installation and climatic separation from the outdoor though air curtains systems is the less contaminating and more efficient option in industrial buildings of the described type.

13/01281 Analysis of compression–absorption cascade refrigeration cycles

Cimsit, C. and Ozturk, I. T. *Applied Thermal Engineering*, 2012, 40, 311–317.

In this study, LiBr–H_2O pair was used for the first time for absorption section of compression–absorption cascade refrigeration cycles. These cycles were analysed theoretically and compared with using different refrigerants in the compression and absorption sections. While LiBr–H_2O and NH_3–H_2O are used as fluid pair in cascade absorption section, R134a, R-410A and NH_3 fluids were used in the vapour compression section of cascade cycle. It was presented that electrical energy consumption in the cascade refrigeration cycle is 48–51% lower than classical vapour compression refrigeration cycles that use R134a, R-410A and NH_3 as working fluids under the same operating conditions, that are an evaporator temperature of 263 K and a condenser temperature of 313 K. Separately the results show that by using LiBr–H_2O pair for absorption section the thermal energy consumption of cascade refrigeration cycle could be reduced by 35% and also general coefficient of performance ($COP_{cyclegen}$) could be improved by 33% compared to the NH_3–H_2O pair.

13/01282 Building markets for energy saving equipment and modelling subsidy strategies in tourism dependent economies

Gravouniotis, P. *et al. Energy Procedia*, 2012, 18, 131–146.

The paper presents selected results of a dynamic non-linear model that simulates critical factors in the diffusion of demand-side energy saving equipment. The modelling exercise is customized to the particular characteristics of the Greek islands of the Aegean Sea. The simulation model in this paper illustrates the impacts and mechanics by which a switch to efficiency can be engineered and its benefits, direct or collateral. It challenges perceptions of planning and has shown so far that a shift to an efficient paradigm is possible within reasonable timeframes. Decisiveness, boldness and consistency seem to be key aspects of the decisions a policy maker needs to take. The search for the diffusion scheme most likely to succeed then needs to iterate a number of scenarios and adopt a specialized appraisal tools. First, a shared vision is critical. A tool such as the one presented in this thesis, can also accommodate the involvement of stakeholders. Indeed, a proper DSM programme and an electricity efficiency plan would need to look at all power consuming services and their evolution in time. Recognizing the limitations of breadth and horizon, the paper provides a new framework under which to consider energy policy decision-making in a localized and customizable way, calling for an intra-sectoral and multi-actor review of a situation in the design of an intervention. A tool expanding from this research could be used, for example, to evaluate the strategy, options, risks and success pathways, along with the inclusion of stakeholders' objectives and concerns.

13/01283 Building resilience to overheating into 1960's UK hospital buildings within the constraint of the national carbon reduction target: adaptive strategies

Short, C. A. *et al. Building and Environment*, 2012, 55, 73–95.

The National Health Service (NHS) Estate in England includes 18.83 Mm^2 of acute hospital accommodation, distributed across 330 sites. Vulnerability to overheating is clear with 15,000 excess deaths occurring nationally during the July 2003 heatwave. The installation of mechanical cooling in existing hospitals appears to be the inevitable recommendation from NHS patient safety risk assessments but the carbon implications would undermine the NHS Carbon Reduction Strategy. NHS CO_2 emissions constitute 25% of all public sector emissions, equivalent to 3% of the UK total. In the post-2008 economic climate, the likelihood of wholesale replacement of the NHS Estate is significantly diminished; refurbishment is now of increasing interest to the Trusts that together make up the NHS. The research project 'Design and Delivery of Robust Hospital Environments in a Changing Climate' seeks to understand the environmental performance of the current NHS Estate and, from this, to establish its resilience. To this end, hospital buildings operated by four NHS Trusts are being monitored and simulated using dynamic thermal models calibrated against measured data. Adaptive refurbishment options are proposed and their relative performance predicted against the existing internal conditions, energy demands and CO_2 emissions. This paper presents findings relating to one representative-type building, a medium-rise ward block dating from the late 1960s. It shows that this particular type may have more resilience in the current climate than might have been expected, that it will remain resilient into the 2030s, and that relatively non-invasive measures would extend and increase its resilience whilst saving energy.

13/01284 Designing net-zero energy buildings for the future climate, not for the past

Robert, A. and Kummert, M. *Building and Environment*, 2012, 55, 150–158.

Net-zero energy buildings (NZEBs) are expected to play an important role in fighting climate change and reducing the energy use of the built environment. But even if the best design practices are widely adopted and implemented, this will only mitigate global warming. It is too late to prevent it. Yet buildings – including net-zero energy buildings – are often designed using historical data representing the average climate between 1961 and 1990, or between 1976 and 2005 at best. This paper investigates the use of the downscaling method known as 'morphing' to generate weather data files. The impact of using these weather files on the energy performance of an actual NZEB is then assessed. Morphing is applied to typical 'horizon years' representative of future climate and also on a month-by-month and year-by-year basis using raw data from a selected GCM. A 50-year series of hourly weather data is obtained and analysed for two different locations, Montréal (QC) and Massena (NY). The data are then used to simulate the performance of a net-zero energy home as it was designed using historical data. The results show that the building misses the net-zero energy target for most years. The year-to-year variability of the total energy use is relatively small but the impact on the energy excess or shortage in relation to the net-zero target is significant. Climate-sensitive buildings such as NZEBs should always be designed using multi-year simulations with weather data that take climate change into account.

13/01285 Feasibility study of a localized residential grey water energy-recovery system

Ni, L. *et al. Applied Thermal Engineering*, 2012, 39, 53–62.

In order to improve the overall efficiency of building energy usage, a grey water energy-recovery system, which adopted a multiple-function heat pump system, was proposed for domestic water heating, and space heating and cooling of buildings. A numerical model has been developed for investigation of annual energy and water consumptions of the proposed system and the conventional building energy system with gas furnace space heating, package air-conditioning, and electricity water heater for hot water heating. Based on a case study of a typical residential house with four family members and three bedrooms in New York city, USA, results show that the overall source energy consumption with the proposed system decreases 33.9% for space heating and cooling and hot water heating, and also the potable water consumption reduces 27.2% compared with those of the conventional system. An extended study with 14 other cities was performed in various climate zones in the USA. Among these 15 cities, the savings in source energy and potable water consumption have ranges of 17–57.9% and 15–34.1%, respectively. The results also show the proposed system can provide substantial energy and potable water savings, particularly with moderate outdoor temperature.

13/01286 Improving energy efficiency in a naphtha reforming plant using Six Sigma methodology

González Falcón, R. *et al. Fuel Processing Technology*, 2012, 103, 110–116.

The distillation process accounts more than 25% of total process energy consumption in refineries. Therefore the energy improvements of the distillations units are very important for this sector. Six Sigma is a methodology supported by a handful of powerful statistical tools in order to reduce variation through continuous process improvement. This paper proposed the application of Six Sigma methodology for improving energy efficiency in a distillation unit of a naphtha reforming plant. The results reproduce the past energy performance of the unit through multivariate models and show optimal operation mode with an expected savings around €150,000 /year. Although the process may further improve optimizing the consumption of the reaction unit.

13/01287 Supply chain management – how can we reduce our energy/climate footprint?

Larsen, H. N. *et al. Energy Procedia*, 2012, 20, 354–363.

This work shows the importance of supply chain management through the use of environmentally extended input–output analysis and life cycle assessment. Results show that for most sectors a majority of the energy/environmental loads are located in the upstream supply chain, both nationally and abroad. Using the tools outlined could therefore help to address important areas to focus the work and guide policies for future energy and emissions reductions. Actions can be at an international policy level, using taxes or other measures to counteract pollution havens, or they could include specific requirements of the products purchased, environmental labelling, or requirements relating to certifications of businesses were products and services are purchased from. The focus of this paper is the public sector, more specifically; the municipalities, where – despite the importance of upstream emissions is identified with a fraction of 90–95% – still most focus is on the 5–10% of the footprint relating to use of heating oil and fuel for transportation.

13/01288 The potential of earth-air heat exchangers for low energy cooling of buildings in south Algeria

Sehli, A. *et al. Energy Procedia*, 2012, 18, 496–506.

A one-dimensional steady numerical model is proposed to estimate the performance of earth-to-air heat exchangers, installed at different depth, used for building cooling/heating. Two parameters are considered to evaluate the performance of the system (Reynolds number and the form factor). With appropriate simplifications, numerical simulation treatment is proposed to predict the temperature fields of the fluids in the pipe and the soil in the proximity of the buried pipe, taking into account meteorological data of south Algeria. Moreover, the agreement with some experimental data available in the literature is very satisfactory.

13/01289 Toward integrated building design: a parametric method for evaluating heating demand

Jaffal, I. *et al. Applied Thermal Engineering*, 2012, 40, 267–274.

This study describes a novel method for evaluating building heating demand based on a statistical approach. The aim is to support integrated building design by providing fast modelling with accuracy close to that of dynamic simulations. A general parametric model encompassing overall building design is proposed based on the analysis of heat transfer. The method is subsequently applied to evaluate the heating demand of a single-family house in a cold French climate. Several polynomial functions are derived from the general model as functions of the amounts of heat transferred by different mechanisms and the physical and geometric building parameters. The model is identified with a small number of dynamic simulations using the design of experiments. The model illustrates how the weighting factors for the various amounts of heat are much higher in cold climates than in hot ones. The authors demonstrate that building heating demand can be accurately analysed using the design parameters of the developed model. This analysis highlights the potential of this approach for supporting building energy designers in the choice of energy-efficient solutions.

17 ENERGY CONVERSION AND RECYCLING

13/01290 Are totally recycled hot mix asphalts a sustainable alternative for road paving?

Silva, H. M. R. D. *et al. Resources, Conservation and Recycling*, 2012, 60, 38–48.

The recycling of reclaimed asphalt pavement (RAP) helps road authorities to achieve their goal of a sustainable road transport system by reducing waste production and resources consumption. The environmental and economic benefits of using RAP in hot mix asphalt (HMA) applications could be pushed up to the limit, by producing totally recycled HMAs (100% RAP), but the performance of this alternative must be satisfactory. In fact, these mixtures could possibly present problems of workability and durability, higher binder aging and low fatigue cracking resistance. Thus, the objective of this study is to determine if totally recycled HMA mixtures could be a good solution for road paving, by evaluating the merit of some rejuvenator agents (commercial product; used engine oil) in improving the aged binders' properties and the recycled mixture performance. Several binder samples were prepared with the mentioned rejuvenators and characterized (Pen, R&B and dynamic viscosity), in order to select the best rejuvenator contents. The production temperatures of the corresponding recycled mixtures were evaluated based on their workability. Totally recycled HMAs were produced with the best previously observed combinations, and their performance (water sensitivity, rutting resistance, stiffness, fatigue resistance, binder aging) was assessed. The main conclusion of this study is that totally recycled HMAs can be a good alternative for road paving, especially if rejuvenator agents are used to reduce their production temperature and to improve their performance.

13/01291 Biogas prediction and design of a food waste to energy system for the urban environment

Curry, N. and Pillay, P. *Renewable Energy*, 2012, 41, 200–209.

Anaerobic digestion applied to the organic waste produced in urban environments could provide a critical solution to growing garbage problems while simultaneously reducing external energy requirements. As landfills across Canada and the rest of the world are filled to their limits, a carbon-neutral process which can locally generate electricity and heat while providing up to 50% volatile solid reduction is something to be seriously considered. This paper investigates the feasibility of urban anaerobic digestion, presents four techniques for biogas estimation – ultimate analysis, yield from molecular formula analysis, a novel computer simulation technique using the Anaerobic Digestion Model #1 and a literature review of experimentally determined biogas yields. In addition, a case study for small-scale anaerobic digestion system design is presented for an urban building.

13/01292 Comparative analysis on waste to energy conversion chains using thermal-chemical processes

Marculescu, C. *et al. Energy Procedia*, 2012, 18, 604–611.

The paper presents the results of theoretical and experimental approach study on solid waste thermal-chemical treatment for power generation. Three main conversion processes were used: direct combustion, pyrolysis and gasification. When applied to large variety of wastes, the option for a certain treatment method (gasification especially due to process low stability) requires the knowledge of physical-chemical characteristics of the waste to be treated. Current debates on cost-effect of these young technologies compared to old incineration are mainly focused on biomass, especially wood under gasification conditions (using air). For atypical waste (MSW, industrial, food industry, farm) operation data or experimental results with respect to process global energy balance are not available for public or the information is restricted to general aspects. The experimental research focused on a large variety of heterogeneous waste (cellulose based, plastic, food industry, agriculture) to energy conversion efficiency. Based on experimental results the electrical power output was estimated for three main conversion chains using the mentioned processes.

13/01293 Effects of discharge recirculation in cooling towers on energy efficiency and visible plume potential of chilling plants

Ge, G. *et al. Applied Thermal Engineering*, 2012, 39, 37–44.

Due to limited space and/or improper placement of evaporative cooling towers, discharge recirculation likely occurs in practical applications. The air recirculation may adversely affect energy efficiency of the chilling plants and increase the potential of visible plume around the towers. In this study, the amount of recirculation in a counter-flow cooling tower is evaluated by computational fluid dynamics (CFD) simulation tests under different enclosure structures and crosswind conditions. Then the effects of recirculation in cooling towers on energy performance of a chilling plant and plume potential are investigated. The evaluation is conducted on a dynamic simulation platform using the weather data in a typical meteorological year of Hong Kong. Results show that crosswind can enhance recirculation in cooling towers under lower air flow rate conditions. The recirculation ratio can reach up to 15%. Results also reveal that air recirculation in cooling towers could result in the increase of overall chilling plant energy consumption by over 1.5%. The recirculation also results in significant increase of plume occurrence frequency, particularly in spring season.

13/01294 Experimental results of gasification of waste tire with air & CO_2, air & steam and steam in a bubbling fluidized bed gasifier

Karatas, H. *et al. Fuel Processing Technology*, 2012, 102, 166–174.

Gasification is one of the thermochemical conversion methods to produce both product gas and solid char. The quality of the product gas widely differs depending on the type of the gasification agent used in the gasification process. Therefore, one of the important parameters in the design phase of the gasification system is the gasification agent. In the present study, a laboratory-scale bubbling fluidized bed gasifier was used to gasify waste tyres with the gasification agents of air and CO_2, air and steam, and steam. Within this frame, the effects of gasification agents, bed material particle size, CO_2 to air ratio, steam to air ratio, steam temperature and steam to fuel ratio on the quality of the product gas were investigated. In order to determine the composition of the product gas, an online gas analyser, which can measure CO, CO_2, CH_4, H_2 and O_2 components, was used. By using the measured gas compositions, the lower heating value (LHV) was calculated to represent the quality of the product gas. Comparing the gasification agents of air and CO_2, air and steam, and steam, the LHV of the product gas was obtained 9.59, 7.34 and 15.21 MJ/Nm^3, respectively. The repetition and uncertainty calculation of the tests were performed.

13/01295 Hydrogen and methane potential based on the nature of food waste materials in a two-stage thermophilic fermentation process

Chu, C. F. *et al. International Journal of Hydrogen Energy*, 2012, 37, (14), 10611–10618.

The purpose of this study is to investigate the biological H_2 and CH_4 potential based on the nature of organic waste materials in a two-stage thermophilic fermentation process. Three varieties of actual waste specifically potato, kitchen garbage and bean curd manufacturing waste (okara) were selected. The production rates for H_2 and CH_4 were as follows: potato, 2.1 and 1.2 l/l/d; garbage, 1.7 and 1.5 l/l/d; okara, 0.4 and 1.4 l/l/d in the continuous processes. The H_2 and CH_4 yields were 20–85 ml H_2/g VS_{added} and 329–364 ml CH_4/g VS_{added}, respectively. The H_2 yield increased and the CH_4 yield decreased in the order of potato, kitchen garbage and okara. The H_2 yield was shown to be not only dependent on the proportion of carbohydrate but also on the hydrolysis pH of the organic waste, which was influenced by the nature of the organic waste materials. Higher yields of H_2 or CH_4 were obtained when the hydrolysis pH of the organic waste was close to the optimum pH range of H_2-producing bacteria or methanogenic archaea in the two-stage fermentation processes.

13/01296 Kinetics studies of synthesis of biodiesel from waste frying oil using a heterogeneous catalyst derived from snail shell

Birla, A. *et al. Bioresource Technology*, 2012, 106, 95–100.

Waste frying oil was used to produce biodiesel using calcined snail shell as a heterogeneous base catalyst. Transesterification reactions were carried out and the yield and conversion of the product were optimized by varying the methanol to oil molar ratio, catalyst amount, reaction temperature, and time. A biodiesel conversion of 99.58% was obtained with a yield of 87.28%. The reaction followed first order kinetics. The activation energy (E_A) was 79 kJ/mol and the frequency factor (A) was 2.98×10^{10} min^{-1}. The fuel properties of the biodiesel were measured according to ASTM D 6751 and found to be within the specifications. Snail shell is a novel source for the production of heterogeneous base catalyst that can be successfully utilized for synthesis of biodiesel of high purity.

13/01297 Parametric optimization and performance analysis of a regenerative organic Rankine cycle using R-123 for waste heat recovery

Roy, J. P. and Misra, A. *Energy*, 2012, 39, (1), 227–235.

This paper presents an analysis of regenerative organic Rankine cycle, based on parametric optimization using R-123 and R-134a during superheating at a constant pressure of 2.50 MPa under realistic conditions. The aim was to select a better working fluid on the basis of obtained system efficiency, turbine work output, irreversibility rate and second law efficiency under applied fixed and variable heat source temperature conditions. R-123 has been found a better working fluid than R-134 for converting low grade heat to power. A computer program has been developed to parametrically optimize and compare the system and second law efficiency, turbine work output, system mass flow rate, irreversibility rate and irreversibility ratio with increases in turbine inlet temperature under different heat source temperature conditions to obtain the optimum operating conditions while using R-123 as the working fluid during superheating at various turbine inlet pressures for the utilization of the waste heat sources of temperatures above 150 °C. The calculated results reveal that an inlet pressure of 2.70 MPa gives the maximum system efficiency, turbine work output and second law efficiency with minimum irreversibility rate, irreversibility ratio and system mass flow rate up to a turbine inlet temperature in the range 165–250 °C.

13/01298 Pyroelectric energy converter for harvesting waste heat: simulations versus experiments

Moreno, R. C. *et al. International Journal of Heat and Mass Transfer*, 2012, 55, (15–16), 4301–4311.

This paper is concerned with numerical simulations of a pyroelectric converter for direct energy conversion of waste heat into electricity. The simulated prototypical device consisted of a hot and cold source separated by a series of vertical microchannels supporting pyroelectric thin films made of co-polymer P(VDF-TrFE) and undergoing the Olsen cycle. A piston was used to vertically oscillate a working fluid back and forth between the thermal sources. The experimental device was instrumented with thermocouples and a pressure sensor. The two-dimensional transient mass, momentum, and energy equations were solved numerically using finite element methods to determine the local and time-dependent temperature at various locations inside the device microchannels. The operating frequency varied from 0.025 to 0.123 Hz and the working fluid was 1.5 or 50 cSt silicone oil. Good agreement was found between the simulated and experimentally measured local mean temperatures for both working fluids at all operating frequencies considered. The local temperature swings were underestimated slightly for 50 cSt silicone oil and significantly more for 1.5 cSt silicone oil. Overall, this study confirms the previous numerical results. Moreover, this numerical model could be used to design and operate the next generation of pyroelectric energy converters based on oscillatory convective heat transfer.

13/01299 Single-chamber bioelectrochemical hydrogen fermentation from garbage slurry

Sasaki, K. *et al. Biochemical Engineering Journal*, 2012, 68, 104–108.

Bioelectrochemical systems (BESs) can control electric flow and resultant microbial activity. The authors designed a single chamber BES to investigate hydrogen production from artificial garbage slurry. A three-electrode system was applied and the potential of the working electrode was regulated to −1.0 V (vs Ag/AgCl). Thus, the potential on the counter electrode was 1.38 V (vs Ag/AgCl). Hydrogen fermentation in the BES was initiated by methanogenic seed sludge. The BES achieved a hydrogen production rate of 2196 $\mathrm{mL\,L^{-1}\,day^{-1}}$ at an organic loading rate of 58.7 g dichromate chemical oxygen demand $\mathrm{L^{-1}\,day^{-1}}$. Acetate and butyrate were the main products, indicating that favourable hydrogen fermentation occurred in the system. Combination of high potential on the counter electrode and relatively low pH condition (5.5–6.4) was effective for constructing hydrogen fermentation even in single chamber system by inhibiting methanogenesis. However, it may be necessary to increase the space between the working and counter electrodes so as to decrease the electrical input. The single-chamber BES could be scaled-up for efficient hydrogen fermentation from garbage slurry.

13/01300 Thermodynamic analysis of alternative refrigeration cycles driven from waste heat in a food processing application

Aneke, M. *et al. International Journal of Refrigeration*, 2012, 35, (5), 1349–1358.

In this paper, the performance comparison of a waste heat driven organic Rankine cycle (ORC) powered vapour compression refrigeration (VCR) system and a waste heat driven NH_3–H_2O absorption refrigeration (AR) system were carried out through modelling and simulation using IPSEpro PSE simulation tool. The simulation result shows that at the given design constraints, the ORC driven VCR system gives a better COP and second law efficiency than the AR system. Also at the breakeven pressure ratio (pressure ratio at which the COP of both system is the same) the ORC driven VCR system also gives a better second law efficiency than the AR system. However, at pressure ratios higher than the breakeven point, performance behaviour seems to contradict the well-known notion that systems with low irreversibility should be more efficient that those with high irreversibility. This is a paradox and might be as a result of a high number of thermal systems in the AR system. However, the trend in the COP and entropy generation obtained for each of the systems conforms to expectation (i.e. increase in COP leads to decrease in entropy generation).

13/01301 Thermodynamic performance assessment of a novel waste heat based triple effect refrigeration cycle

Agrawal, B. K. and Karimi, M. N. *International Journal of Refrigeration*, 2012, 35, (6), 1647–1656.

In the proposed triple effect refrigeration cycle, a natural refrigerant based N_2O compression cycle is employed to the combined absorption cycle with an ejector refrigeration cycle. This triple effect cycle combines the advantages of absorption cycle, ejector cycle and low temperature N_2O refrigerant based compression cycle. This combined cycle could produce refrigeration output of different magnitude at different temperature simultaneously and could be driven by the waste heat which is available abundantly in different form. System performance and exergy destruction on each component of combined cycle are evaluated based on parametric, energetic and exergetic analysis. The results show that the waste flue gas temperature, turbine inlet pressure, turbine outlet pressure, ejector evaporator temperature and compressor discharge pressure have significant effects on the refrigeration outputs, exergy efficiency and thermal efficiency.

13/01302 Transesterification of edible, non-edible and used cooking oils for biodiesel production using calcined layered double hydroxides as reusable base catalysts

Sankaranarayanan, S. *et al. Bioresource Technology*, 2012, 109, 57–62.

Fatty acid methyl esters (FAME) were produced from edible, non-edible and used cooking oils with different fatty acid contents by transesterification with methanol using calcined layered double hydroxides (LDHs) as solid base catalysts. Among the catalysts, calcined CaAl2-LDH (hydrocalumite) showed the highest activity with >90% yield of FAME using low methanol:oil molar ratio (<6:1) at 65 °C in 5 h. The activity of the catalyst was attributed to its high basicity as supported by Hammett studies and CO_2-TPD measurements. The catalyst was successfully reused in up to four cycles. Some of the properties such as density, viscosity, neutralization number and glycerol content of the obtained biodiesel matched well with the standard DIN values. It is concluded that a scalable heterogeneously catalysed process for production of biodiesel in high yields from a wide variety of triglyceride oils including used oils is possible using optimized conditions.

13/01303 Waste heat recovery from a landfill gas-fired power plant

Gewald, D. *et al. Renewable and Sustainable Energy Reviews*, 2012, 16, (4), 1779–1789.

Waste treatment and management is a certain challenge especially in areas with high population density. One of the options for waste treatment is landfilling, where the amount of municipal waste also produces landfill gas through anaerobic digestion. The heating value of the landfill gas is high enough to use it as a fuel in combustion processes, e.g. in internal combustion engines (ICEs) to produce electric power. In Ano Liosia, Athens, Greece up to 6000 tons of waste are landfilled every day and the landfill gas is used in an ICE power station directly at the site of the landfill. The power station consists of 15 ICEs and has an installed capacity of 23.5 MW. The major advantages of using ICE for power generation are the high electrical efficiency of ICEs and their fast load response. However, more than 50% of the landfill gas energy content is still released to the atmosphere as engine waste heat (exhaust gas and engine cooling water). The aim of this paper is to study the possibilities of using this large amount of heat in order to increase the electricity production and efficiency of the Ano Liosia power station. Therefore, a thermodynamic and economic analysis of two different waste heat recovery systems is conducted. The water/steam cycle and the organic Rankine cycle are examined and evaluated by means of thermodynamic cycle simulation and by calculating their specific costs of power generation. Their advantages and disadvantages considering their application in landfill gas-fired ICE power stations are discussed under the consideration of maximal thermodynamic efficiency and minimal costs of power generation.

13/01304 Waste management strategy focused on maintenance, storage and recycling

Someya, Y. *et al. Fusion Engineering and Design*, 2012, 87, (7–8), 1282–1285.

Waste is generated at the moment when the operation of a fusion reactor is halted and maintenance is started for periodic replacement of blanket modules and divertor. Used blanket and divertor need to be replaced shortly after the shutdown for high plant availability, as long as high surface dose rate and decay heat of the blanket and divertor can be handled. In this sense, nuclear characteristics of the blanket and divertor need to be understood for a reasonable maintenance scheme. For the purpose, neutronic calculations were carried out on the blanket and divertor using a THIDA-2 code with FENDL-2.0. For a SlimCS DEMO reactor, the calculated decay heat for each 1/12-sector was as high as 5 MW just after the shutdown and 0.3 MW one month later. For the maintenance, a cooled shielding structure (CSS) was proposed to remove the decay heat and to shield gamma-rays from the sector. When maintenance is done one month after the shutdown, the sector temperature is maintained to be 550 °C or lower with the cooling by the CSS of 50 °C. In order to avoid tritium release from the sector during the maintenance, a cask should be used to transport the sector. For efficient use of resources, breeding and neutron multiplying materials should be reused or recycled. A possible strategy for reuse or recycle is also presented.